

Noble

Access DB# 146293

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: BEN SACKY Examiner #: 73489 Date: 2/28/05
Art Unit: 1626 Phone Number 302-0704 Serial Number: 101049,725
Mail Box and Bldg/Room Location: REM 5B3 Results Format Preferred (circle): PAPER DISK E-MAIL

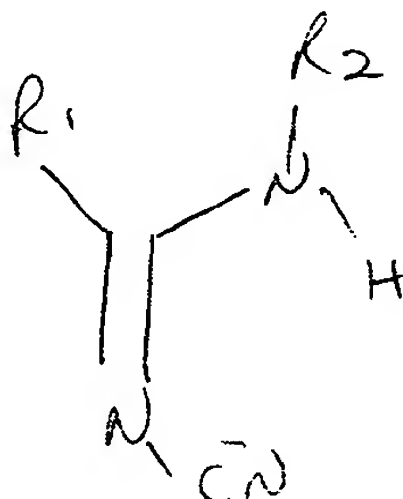
If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Substituted n-glycine amidines
Inventors (please provide full names): Fesung et al.

Earliest Priority Filing Date: _____

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*



R₁ and R₂ are as defined in claims 1 and two.

Thanks

STAFF USE ONLY

| | Type of Search | Vendors and cost where applicable |
|--|------------------------|-----------------------------------|
| Searcher: <u>Noble</u> | NA Sequence (#) _____ | STN <u>531</u> |
| Searcher Phone #: _____ | AA Sequence (#) _____ | Dialog _____ |
| Searcher Location: _____ | Structure (#) <u>2</u> | Questel/Orbit _____ |
| Date Searcher Picked Up: _____ | Bibliographic <u>✓</u> | Dr.Link _____ |
| Date Completed: <u>3/8/05</u> | Litigation _____ | Lexis/Nexis _____ |
| Searcher Prep & Review Time: <u>10</u> | Fulltext _____ | Sequence Systems _____ |
| Clerical Prep Time: _____ | Patent Family _____ | WWW/Internet _____ |
| Online Time: <u>10</u> | Other _____ | Other (specify) _____ |



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 146293

TO: Ben Sackey
Location: 5c31/5c18
Art Unit: 1626
Tuesday, March 08, 2005

Case Serial Number: 10/04972⁵

From: Noble Jarrell
Location: Biotech-Chem Library
Rem 1B71
Phone: 272-2556

Noble.jarrell@uspto.gov

Search Notes

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(FILE 'HOME' ENTERED AT 07:28:20 ON 08 MAR 2005)

FILE 'REGISTRY' ENTERED AT 07:28:24 ON 08 MAR 2005

L1 STR
L2 13 L1
L3 297 L1 FULL
SAV TEM L3 SAC725F0/A

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E GESING E/AU
L5 104 E4-10
E HENSE A/AU
L6 12 E3-4
E KATHER K/AU
L7 42 E3.E5
E LEHR S/AU
L8 92 E3.E9-11
E RIEBEL H/AU
L9 321 E3-14
E ROHE L/AU
L10 45 E3-4
E VOIGT K/AU
L11 291 E3-5.E15
E DREWES M/AU
L12 250 E3-8
E FEUCHT D/AU
L13 172 E3.E6
E PONTZEN R/AU
L14 134 E3-4
E WETCHOLOWSKY I/AU
L15 61 E3-4
L16 52 L3
L17 3 L16 AND L4-15
L18 49 L16 NOT L17

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L19 0 L3

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L21 42 L18 AND L20
SEL HIT RN L21

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SEL RN 11-49 56-87 89 91-125 127-153 159-164
L23 140 E233-372

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L24 18 L23 AND L21

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FILE 'REGISTRY' ENTERED AT 07:58:42 ON 08 MAR 2005

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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Property values tagged with IC are from the ZIC/VINITI data file
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Search done by Noble Jarrell

STRUCTURE FILE UPDATES: 6 MAR 2005 HIGHEST RN 843607-47-6
DICTIONARY FILE UPDATES: 6 MAR 2005 HIGHEST RN 843607-47-6

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

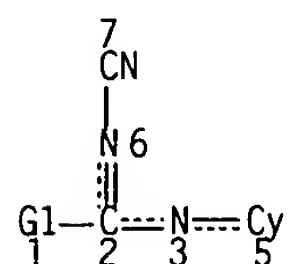
Please note that search-term pricing does apply when
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> d que sta l3

L1 STR



VAR G1=H/AK/CY

NODE ATTRIBUTES:

CONNECT IS E2 RC AT 3

CONNECT IS E2 RC AT 6

DEFAULT MLEVEL IS ATOM

GGCAT IS PCY AT 5

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 6

STEREO ATTRIBUTES: NONE

L3 297 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 16771 ITERATIONS

297 ANSWERS

SEARCH TIME: 00.00.49

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FILE 'HCAPLUS' ENTERED AT 07:58:51 ON 08 MAR 2005

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FILE COVERS 1907 - 8 Mar 2005 VOL 142 ISS 11

Search done by Noble Jarrell

FILE LAST UPDATED: 7 Mar 2005 (20050307/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L17 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 2005:76262 HCAPLUS
 DN 142:176835
 ED Entered STN: 28 Jan 2005
 TI Preparation of 3-phenyl-2-pyrazolines as PAR-1 antagonists for treatment of cardiovascular diseases
 IN Allerheiligen, Swen; Brohm, Dirk; Diedrichs, Nicole; Froehlen, Britta-Nicole; Gerdes, Christoph; Gnoth, Mark Jean; Heckroth, Heike; Huebsch, Walter; Perzborn, Elisabeth; Stahl, Elke; Voehringer, Verena
 PA Bayer Healthcare A.-G., Germany
 SO PCT Int. Appl. 183 pp.
 CODEN: PIXXD2
 DT Patent
 LA German
 IC ICM A61K031-4155
 ICS A61P009-00; C07D403-04; C07D409-14; C07D405-14; C07D401-14; C07D413-04; C07D417-04; C07D403-14; C07D401-04; C07D417-14; C07D413-14
 CC 28-8 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1. 63

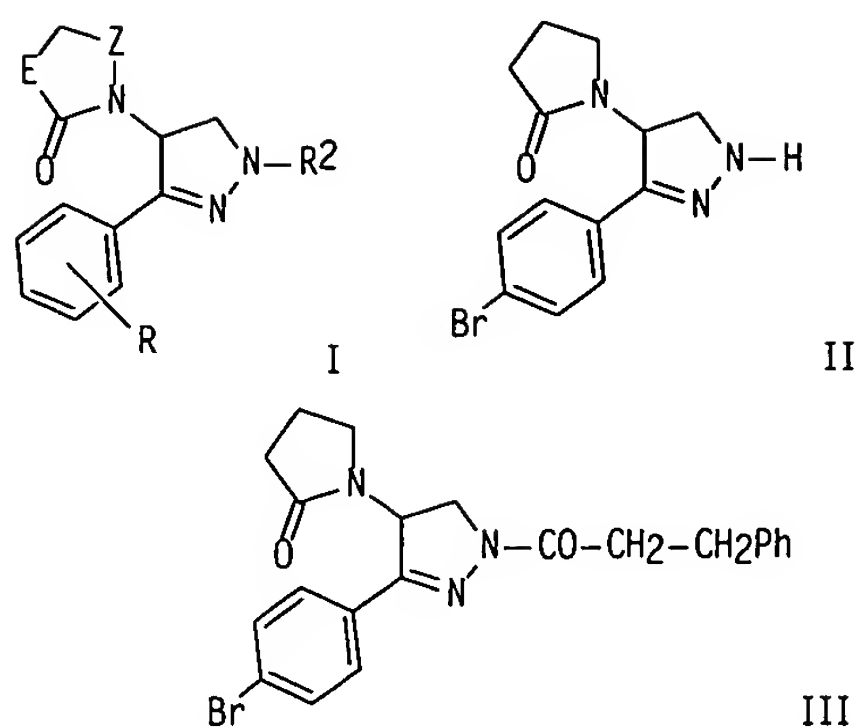
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---|------|----------|-----------------|----------|
| WO 2005007157 | A1 | 20050127 | WO 2004-EP7227 | 20040702 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG DE 102004010545 A1 20050224 DE 2004-102004010545 20040304 PRAI DE 2003-10331951 A 20030715 DE 2004-102004010545 A 20040304 | | | | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|---------------|-------|--|
| WO 2005007157 | ICM | A61K031-4155 |
| | ICS | A61P009-00; C07D403-04; C07D409-14; C07D405-14; C07D401-14; C07D413-04; C07D417-04; C07D403-14; C07D401-04; C07D417-14; C07D413-14 |

GI



- AB Title compds. I [R = (R1)m; Z = (CH2)n; m = 0-3; n = 1-3; R1 = halo, OH, NH2, etc.; E = CH2, NH, O, etc.; R2 = COX, CONHY, CSNHY, etc.; X = R3, fluoro-substituted alkylen-R4; Y = R3, fluoro-substituted alkylen-R4; R3 = 1,3-benzodioxol, 2,2-difluoro-1,3-benzodioxol, 2,3-dihydro-1,4-benzodioxin, etc.; R4 = H, 1,3-benzodioxol, 2,2-difluoro-1,3-benzodioxol, etc.] and their pharmaceutically acceptable salts and formulations were prepared For example, 3-phenylpropionyl chloride N-acylation of pyrazole II, e.g., prepared from 4-bromophenacyl bromide in 2-steps, afforded phenylpyrazoline III in 72% yield. In PAR-1 antagonist assays, 10-examples of compds. I exhibited IC50 values ranging from 2-220 nM. Compds. I are claimed to be useful for the treatment of cardiovascular and thromboembolic diseases.
- ST phenylpyrazoline prepn PAR1 antagonist; cardiovascular agent prepn PAR1 antagonist; antithrombotic agent prepn PAR1 antagonist
- IT Thrombin receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(PAR-1 (proteinase-activated receptor 1); preparation of phenylpyrazolines as PAR-1 antagonists for treatment of cardiovascular diseases)
- IT Proteinase-activated receptors
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(PAR-1; preparation of phenylpyrazolines as PAR-1 antagonists for treatment of cardiovascular diseases)
- IT Cardiovascular agents
Human
(preparation of phenylpyrazolines as PAR-1 antagonists for treatment of cardiovascular diseases)
- IT Embolism
(thromboembolism, treatment of; preparation of phenylpyrazolines as PAR-1 antagonists for treatment of cardiovascular diseases)
- IT Anticoagulants
Cardiovascular system, disease
(treatment of; preparation of phenylpyrazolines as PAR-1 antagonists for treatment of cardiovascular diseases)
- IT 153337-19-0P 179537-57-6P 179537-60-1P 832748-23-9P 832748-24-0P
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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(preparation of phenylpyrazolines as PAR-1 antagonists for treatment of
cardiovascular diseases)

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RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of phenylpyrazolines as PAR-1 antagonists for treatment of
 cardiovascular diseases)

IT 50-00-0, Formaldehyde, reactions 64-04-0, (2-Phenylethyl)amine
 77-78-1, Dimethylsulfate 99-73-0 106-47-8, 4-Chloroaniline, reactions
 107-85-7, 3-Methylbutan-1-amine 108-91-8, Cyclohexylamine, reactions
 109-73-9, Butylamine, reactions 110-58-7, n-Pentylamine 140-77-2,
 Cyclopentanepropanoic acid 143-33-9, Sodium cyanide 403-29-2
 460-39-9, 3,3,3-Trifluoropropan-1-amine 497-25-6, 1,3-Oxazolidin-2-one
 530-62-1 536-38-9 616-45-5, 2-Pyrrolidinone 645-45-4,
 3-Phenylpropionyl chloride 1505-47-1, 4-Thiophenbutanoic acid
 1943-82-4, (2-Isocyanatoethyl)benzene 2038-57-5, 3-Phenylpropan-1-amine
 2525-62-4, Hexylisocyanate 2706-56-1, (2-Pyridin-2-ylethyl)amine
 3218-02-8, 1-Cyclohexylmethanamine 4441-63-8, Cyclohexanebutanoic acid
 5391-39-9, 1-Acetylimidazolidin-2-one 5452-35-7, Cycloheptylamine
 7803-57-8, Hydrazine hydrate 13078-79-0, 2-(3-Chlorophenyl)ethanamine
 13078-80-3, 2-(2-Chlorophenyl)ethylamine 17247-58-4,
 Bromomethylcyclobutane 22236-10-8, 4-Difluoromethoxyphenylamine
 30433-91-1, 2-(2-Thienyl)ethanamine 34857-66-4 39479-97-5
 39825-36-0, Isopropyl-.beta.-alaninate 54303-30-9,
 2-(Ethylmercapto)ethylamine Hydrochloride 55204-93-8,
 2-Chlorobenzylisocyanate 59311-67-0, 2-(3-Thienyl)ethanamine
 75653-86-0, 3-(1H-Pyrazol-1-yl)propan-1-amine 79463-77-7 832753-65-8,
 3-[(4-tert-Butylcyclohexyl)oxy]propan-1-amine 832753-69-2,
 1-[3-(Trifluoromethyl)cyclohexyl]methanamine

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of phenylpyrazolines as PAR-1 antagonists for treatment of
 cardiovascular diseases)

IT 4426-03-3P, Cyclobutylacetoneitrile 43003-15-2P 60637-97-0P,
 2-Cyclobutylethylamine 148668-51-3P 148668-54-6P 153337-72-5P
 153337-77-0P, 1-[3-(4-Fluorophenyl)-4,5-dihydro-1H-pyrazol-4-yl]pyrrolidin-
 2-one 470477-87-3P, 5-Methoxy-3,4-dihydro-2H-pyrrole 832753-10-3P,
 1-[2-(4-Bromophenyl)-2-oxoethyl]pyrrolidin-2-one 832753-13-6P,
 1-[2-(4-Fluorophenyl)-2-oxoethyl]pyrrolidin-2-one 832753-16-9P
 832753-18-1P 832753-20-5P 832753-22-7P 832753-24-9P 832753-27-2P,
 3-[2-(4-Bromophenyl)-2-oxoethyl]-1,3-oxazolidin-2-one 832753-29-4P,
 1-Acetyl-3-[2-(4-bromophenyl)-2-oxoethyl]imidazolidin-2-one 832753-35-2P
 832753-37-4P 832753-39-6P 832753-41-0P 832753-44-3P 832753-46-5P
 832753-47-6P, 1-[1-(4-Chlorobenzoyl)vinyl]pyrrolidin-2-one 832753-51-2P
 832753-53-4P 832753-56-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of phenylpyrazolines as PAR-1 antagonists for treatment of
 cardiovascular diseases)

RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Ahn, H; DRUGS OF THE FUTURE 2001, V26(11), P1065 HCAPLUS

(2) Bayer Ag; EP 0529451 A 1993 HCAPLUS

(3) Bayer Ag; EP 0532918 A 1993 HCAPLUS

- (4) Bayer Ag; EP 0591780 A 1994 HCAPLUS
 (5) Erdelen, C; WO 9324463 A 1993 HCAPLUS
 (6) Rohm & Haas; EP 0466408 A 1992 HCAPLUS

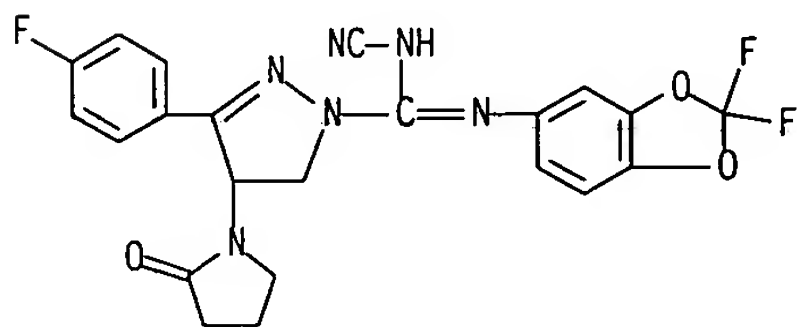
IT 832749-33-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
 (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
 (Uses)

(preparation of phenylpyrazolines as PAR-1 antagonists for treatment of
 cardiovascular diseases)

RN 832749-33-4 HCAPLUS

CN 1H-Pyrazole-1-carboximidamide, N-cyano-N'-(2,2-difluoro-1,3-benzodioxol-5-
 yl)-3-(4-fluorophenyl)-4,5-dihydro-4-(2-oxo-1-pyrrolidiny)- (9CI) (CA
 INDEX NAME)



L17 ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:807725 HCAPLUS

DN 133:350059

ED Entered STN: 16 Nov 2000

TI Herbicidal N-cyano-amidines

IN Gesing, Ernst R. F.; Hense, Achim; Kather,
 Kristian; Lehr, Stefan; Riebel, Hans-Jochem;
 Rohe, Lothar; Voigt, Katharina; Drewes, Mark Wilhelm;
 Feucht, Dieter; Pontzen, Rolf; Wetcholowsky,
 Ingo

PA Bayer A.-G., Germany

SO Ger. Offen., 14 pp.

CODEN: GWXXBX

DT Patent

LA German

IC ICM C07C261-04

ICS A01N047-40; C07D215-38; C07D221-04; C07D333-50; C07D335-06;
 C07D311-04

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 5

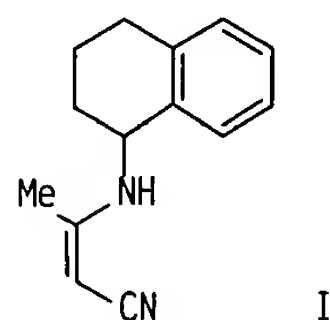
FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|--|------|----------|------------------|----------|
| DE 19921886 | A1 | 20001116 | DE 1999-19921886 | 19990512 |
| CA 2373429 | AA | 20001123 | CA 2000-2373429 | 20000504 |
| WO 2000069813 | A1 | 20001123 | WO 2000-EP4013 | 20000504 |
| W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | | | | |
| RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | | | | |
| BR 2000010447 | A | 20020213 | BR 2000-10447 | 20000504 |
| EP 1178956 | A1 | 20020213 | EP 2000-929495 | 20000504 |
| R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO | | | | |

| | | | | |
|-----------------------|----|----------|----------------|----------|
| JP 2002544255 | T2 | 20021224 | JP 2000-618230 | 20000504 |
| AU 765922 | B2 | 20031002 | AU 2000-47553 | 20000504 |
| PRAI DE 1999-19921886 | A | 19990512 | | |
| WO 2000-EP4013 | W | 20000504 | | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|----------------------|-------|---|
| DE 19921886 | ICM | C07C261-04 |
| | ICS | A01N047-40; C07D215-38; C07D221-04; C07D333-50; C07D335-06; C07D311-04 |
| DE 19921886 | ECLA | A01N047/40; C07C261/04; C07D333/54B |
| OS MARPAT 133:350059 | | |
| GI | | |



AB N-Cyano-amidines R₂NHCR₁:NCN [R₁ = H, (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl; R₂ = (un)substituted benzannellated, pyridoannellated, thienoannellated cycloalk(en)yl, oxacycloalk(en)yl or thiacycloalk(en)yl] were prepared for use as herbicides. Thus, NCN:CM₂OMe was treated with 1,2,3,4-tetrahydro-1-naphthylamine to give the cyano amidine I. I was effective in both pre- and post-emergence tests.

ST cyano amidine prepn herbicide

IT Herbicides
(preparation of herbicidal N-cyano-amidines)

IT **306284-52-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of herbicidal N-cyano-amidines)

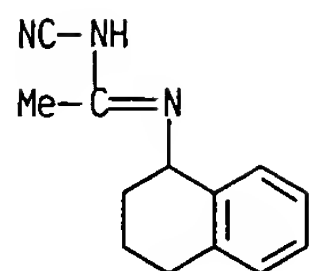
IT **255374-61-9P 255374-62-0P 255374-63-1P 255374-64-2P 255374-65-3P 255374-66-4P 306284-53-7P 306284-54-8P 306284-55-9P 306284-56-0P 306284-57-1P 306284-58-2P 306284-59-3P 306284-60-6P 306284-61-7P 306284-62-8P 306284-63-9P 306284-64-0P 306284-65-1P 306284-66-2P 306284-67-3P 306284-68-4P 306284-69-5P 306284-70-8P**
RL: AGR (Agricultural use); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of herbicidal N-cyano-amidines)

IT 2217-40-5, 1,2,3,4-Tetrahydro-1-naphthylamine 5652-84-6
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of herbicidal N-cyano-amidines)

IT **306284-52-6P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of herbicidal N-cyano-amidines)

RN 306284-52-6 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(1,2,3,4-tetrahydro-1-naphthalenyl)- (9CI) (CA INDEX NAME)



L17 ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 2000:54236 HCAPLUS

DN 132:107782

ED Entered STN: 23 Jan 2000

TI Preparation of N-arylalkylimidamides as pesticides

IN Riebel, Hans-Jochem; Gerdes, Peter; Gesing, Ernst Rf.;
Hense, Achim; Kanellakopulos, Johannes; Kather, Kristian
; Kirsten, Rolf; Lehr, Stefan; Rohe, Lothar; Voigt,
Katharina; Wollweber, Detlef; Andersch, Wolfram

PA Bayer A.-G., Germany

SO Ger. Offen., 66 pp.

CODEN: GWXXBX

DT Patent

LA German

IC ICM C07C261-04

ICS C07C323-32; C07C317-32; C07C257-22; A01N037-52; C07D333-04;
C07D325-00; C07D315-00; C07D277-22

CC 25-19 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 5

FAN.CNT 1

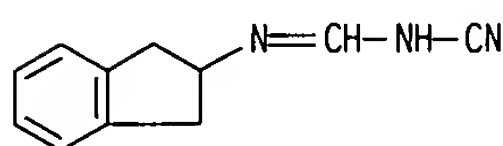
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|------------------|------|----------|---|----------|
| PI | DE 19924273 | A1 | 20000120 | DE 1999-19924273 | 19990527 |
| | CA 2337773 | AA | 20000127 | CA 1999-2337773 | 19990707 |
| | WO 2000003976 | A1 | 20000127 | WO 1999-EP4747 | 19990707 |
| | W: | | | AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM | |
| | RW: | | | GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG | |
| | AU 9951573 | A1 | 20000207 | AU 1999-51573 | 19990707 |
| | BR 9912242 | A | 20010410 | BR 1999-12242 | 19990707 |
| | EP 1097128 | A1 | 20010509 | EP 1999-936489 | 19990707 |
| | EP 1097128 | B1 | 20040512 | | |
| | R: | | | AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI | |
| | JP 2002520385 | T2 | 20020709 | JP 2000-560085 | 19990707 |
| | AT 266631 | E | 20040515 | AT 1999-936489 | 19990707 |
| | ES 2221407 | T3 | 20041216 | ES 1999-936489 | 19990707 |
| | EG 22587 | A | 20030430 | EG 1999-863 | 19990715 |
| | US 6638979 | B1 | 20031028 | US 2001-743588 | 20010205 |
| PRAI | DE 1998-19832447 | A1 | 19980718 | | |
| | DE 1999-19924273 | A | 19990527 | | |
| | WO 1999-EP4747 | W | 19990707 | | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|-------------|-------|---|
| DE 19924273 | ICM | C07C261-04 |
| | ICS | C07C323-32; C07C317-32; C07C257-22; A01N037-52; C07D333-04; C07D325-00; C07D315-00; C07D277-22 |
| DE 19924273 | ECLA | A01N047/40; C07C261/04; C07C317/46; C07C323/41; |

C07D277/64; C07D307/81; C07D313/12; C07D317/5;
 C07D321/12; C07D333/20; C07D333/28
 WO 2000003976 ECLA A01N047/40; C07D321/12; C07D333/20; C07D333/28;
 C07C261/04; C07C317/46; C07C323/41; C07D277/6;
 C07D307/81; C07D313/12; C07D317/58
 US 6638979 ECLA A01N047/40; C07C317/46; C07C323/41; C07D277/64;
 C07D307/81; C07D313/12; C07D317/58; C07D321/1;
 C07D333/20; C07D333/28; C07C261/04
 OS MARPAT 132:107782
 AB RNH:CR1NR2R3 [R = cyano or N02; R1 = H, (cyclo)alkyl, Ph, etc.; R2 = H,
 (cyclo)alkyl, etc.; R3 = CR4R5XR6, YR7, OR8; R4,R5 = H or (un)substituted
 (cyclo)alkyl; R6,R7 = aryl, cycloalk(en)yl, non-N-containing heterocyclyl,
 etc.; R8 = alkyl or (un)substituted aryl; X = bond alkylene(oxy), etc.; Y
 = bond oxyalkylene, etc.] were prepared Thus, (R)-H2NCHMeC6H4Cl-4 was
 amidated by MeC(:NCN)OMe to give (R)-NCN:CMenHCHMeC6H4Cl-4 (I). Data for
 nematocidal activity of I were given.
 ST arylalkylimidamide prepn pesticide
 IT Pesticides
 (N-arylalkylimidamides)
 IT Acaricides
 Insecticides
 Nematocides
 (preparation of N-arylalkylimidamides as pesticides)
 IT 255372-55-5P 255372-56-6P 255372-57-7P 255372-58-8P 255372-59-9P
 255372-60-2P 255372-61-3P 255372-62-4P 255372-63-5P 255372-64-6P
 255372-65-7P 255372-66-8P 255372-67-9P 255372-68-0P 255372-69-1P
 255372-70-4P 255372-71-5P 255372-72-6P 255372-73-7P 255372-74-8P
 255372-76-0P 255372-77-1P 255372-78-2P 255372-79-3P 255372-80-6P
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 255374-70-0P 255374-71-1P 255374-72-2P 255374-73-3P

255374-74-4P 255374-75-5P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of N-arylalkylimidamides as pesticides)
 IT 27298-99-3, (R)-4-Chloro-.alpha.-methylbenzenemethanamine
 RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of N-arylalkylimidamides as pesticides)
 IT 255374-61-9P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of N-arylalkylimidamides as pesticides)
 RN 255374-61-9 HCAPLUS
 CN Methanimidamide, N-cyano-N'-(2,3-dihydro-1H-inden-2-yl)- (9CI) (CA INDEX NAME)



=> d all hitstr 124 tot

L24 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1996:513746 HCAPLUS
 DN 125:157769
 ED Entered STN: 28 Aug 1996
 TI Synthesis and Selective Coronary Vasodilatory Activity of 3,4-Dihydro-2,2-bis(methoxymethyl)-2H-1-benzopyran-3-ol Derivatives: Novel Potassium Channel Openers
 AU Cho, Hidetsura; Katoh, Susumu; Sayama, Shinsuke; Murakami, Kengo; Nakanishi, Hiroyuki; Kajimoto, Yasuyuki; Ueno, Hiroshi; Kawasaki, Hisashi; Aisaka, Kazuo; Uchida, Itsuo
 CS Central Pharmaceutical Research Institute, Japan Tobacco Inc., Takatsuki, 569, Japan
 SO Journal of Medicinal Chemistry (1996), 39(19), 3797-3805
 CODEN: JMCMAR; ISSN: 0022-2623
 PB American Chemical Society
 DT Journal
 LA English
 CC 1-3 (Pharmacology)
 Section cross-reference(s): 27
 AB A variety of compds. having a benzopyran such as levcromakalim generally exhibit potent antihypertensive activity. During extensive investigations aimed toward identifying K⁺ channel openers having selective coronary vasodilation without potent hypotensive and tachycardia effects, we synthesized a series of 3,4-dihydro-2H-1-benzopyran-3-ol derivs. modified at positions 2, 4, and 6 in the benzopyran ring. Initially, compds. having two methoxymethyl groups at position 2 were found to show a selective effect on coronary blood flow (CoBF) relative to mean arterial pressure (MAP) in anesthetized dogs. To find more potent vasodilators, various benzopyran derivs. modified at position 4 were synthesized and structure-activity relationships were examined by evaluation of the extent and duration of the increase in CoBF in anesthetized dogs. As a result, compds. having a (1,6-dihydro-6-oxopyridazin-3-yl)amino group at position 4, in addition to the two methoxymethyl groups at position 2, were found to be more potent and to have an improved duration of action. Among these compds., JTV-506, (-)-(3S,4R)-6-cyano-3,4-dihydro-4-[(1,6-dihydro-1-methyl-6-oxopyridazin-3-yl)amino]-2,2-bis(methoxymethyl)-2H-1-benzopyran-3-ol, exhibited good selectivity for its effect. Administration of this compound

(0.03 mg/kg, po) elicited an increase of CoBF without a change of systemic blood pressure and heart rate (HR) in conscious dogs. Further evaluation was performed with respect to (i) the selectivity of its action on the coronary artery vs. the aorta and (ii) its effects on MAP, HR, and electrocardiogram. ST elevation. As a result, JTV-506 was selected as a potent and selective coronary vasodilator with various pharmacological features favoring clinical development.

ST benzopyranol deriv prepn coronary vasodilator

IT Vasodilators

(coronary, preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT Ion channel openers

(potassium, preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT Molecular structure-biological activity relationship

(vasodilating, preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT 149342-19-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT 170148-35-3P 170148-36-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT 168819-36-1P 168819-41-8P 168819-44-1P

168819-52-1P 168819-55-4P 168819-64-5P 168819-80-5P

169273-23-8P 170148-29-5P 170148-30-8P 170148-41-1P

170148-42-2P 170148-44-4P 170148-59-1P 170148-61-5P 170148-65-9P

170148-67-1P 170148-76-2P 170148-77-3P 170148-78-4P 170148-79-5P

170148-80-8P 170148-81-9P 170148-82-0P 170148-85-3P 170148-87-5P

170148-88-6P 170148-90-0P 170148-91-1P 170148-99-9P 170149-04-9P

170149-06-1P 180307-04-4P 180307-05-5P 180307-06-6P

180307-07-7P 180307-08-8P 180307-09-9P 180470-15-9P

180470-16-0P 180470-17-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT 103-71-9, Phenyl isocyanate, reactions 106-94-5 586-75-4,

p-Bromobenzoyl chloride 623-69-8, 1,3-Dimethoxypropan-2-ol 5436-01-1

5469-69-2, 3-Amino-6-chloropyridazine 10400-19-8, Nicotinoyl chloride

13506-28-0 35794-84-4, 5-Cyano-2-hydroxyacetophenone 41835-08-9,

N-Cyano-N'-phenylthiourea 57041-95-9 168819-61-2 180307-10-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT 18664-32-9P, 1,3-Dimethoxypropan-2-one 168819-11-2P 168819-12-3P

168819-13-4P 168819-65-6P 168819-66-7P 168819-67-8P 169102-75-4P

169102-76-5P 169102-78-7P 170148-33-1P 170149-21-0P 180470-18-2P

180470-19-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

IT 149342-19-8

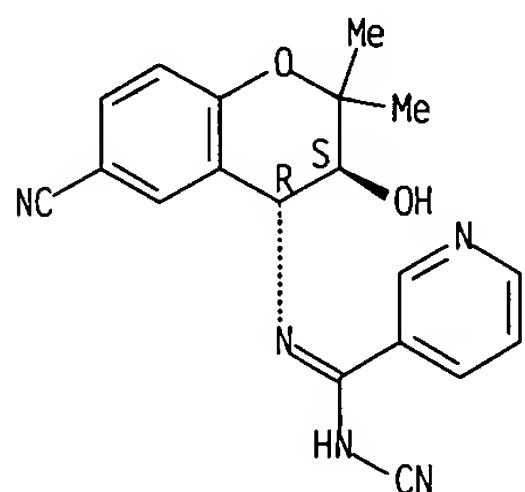
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

RN 149342-19-8 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT 168819-36-1P 168819-41-8P 168819-44-1P

168819-64-5P 168819-80-5P 169273-23-8P

180307-04-4P 180307-05-5P 180470-15-9P

180470-17-1P

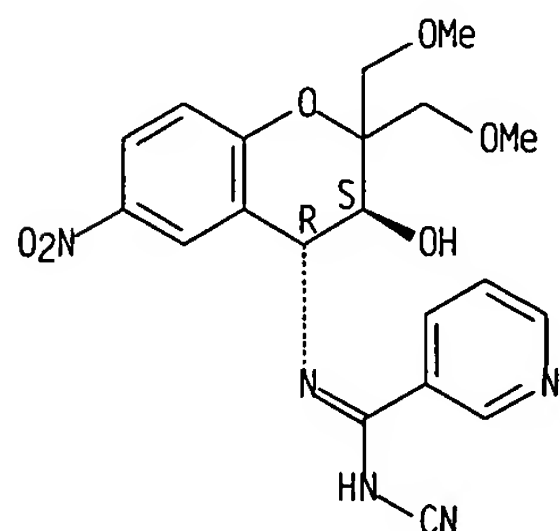
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and selective coronary vasodilatory activity of dihydrobis(methoxymethyl)benzopyranol derivs.: novel potassium channel openers)

RN 168819-36-1 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

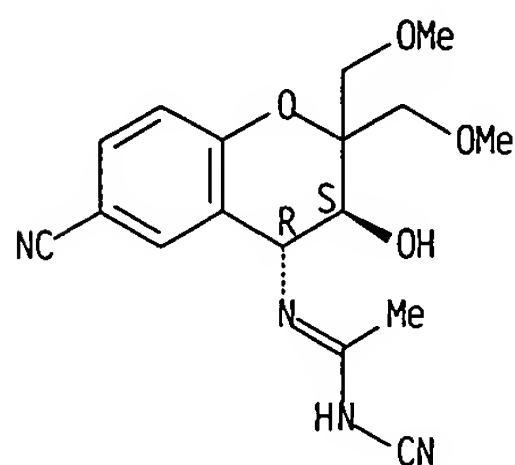
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-41-8 HCAPLUS

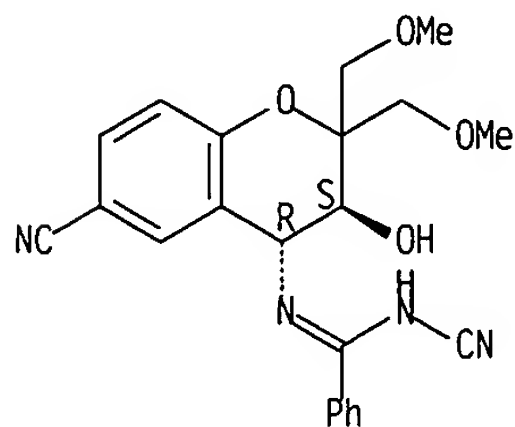
CN Ethanimidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

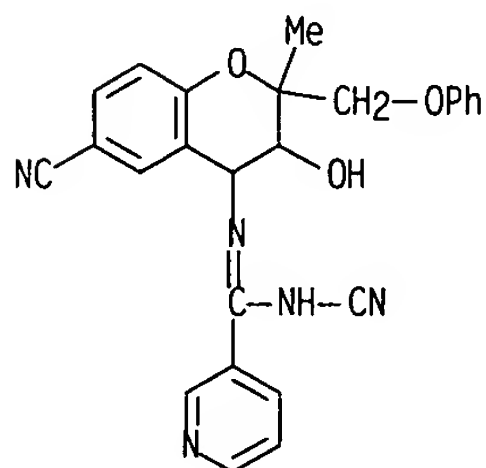


RN 168819-44-1 HCAPLUS
CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

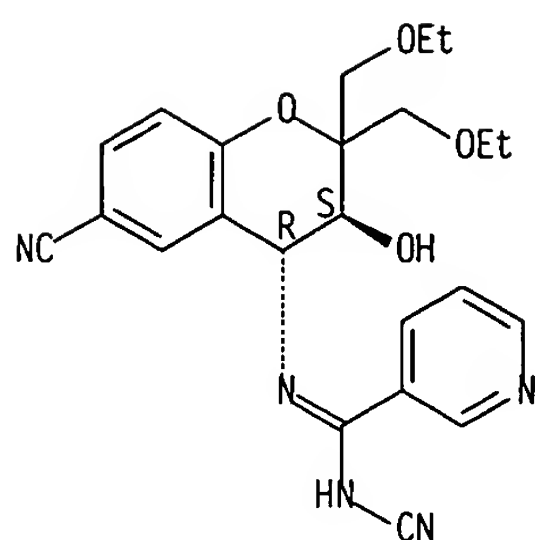


RN 168819-64-5 HCAPLUS
CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-methyl-2-(phenoxymethyl)-2H-1-benzopyran-4-yl]- (9CI) (CA INDEX NAME)



RN 168819-80-5 HCAPLUS
CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-2,2-bis(ethoxymethyl)-3,4-dihydro-3-hydroxy-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

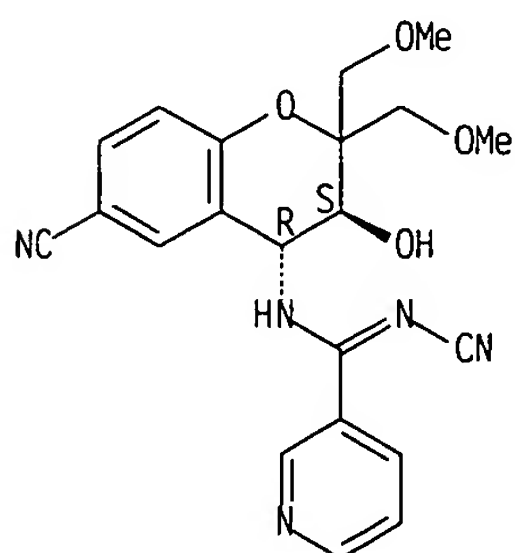
Absolute stereochemistry.
Double bond geometry unknown.



RN 169273-23-8 HCAPLUS

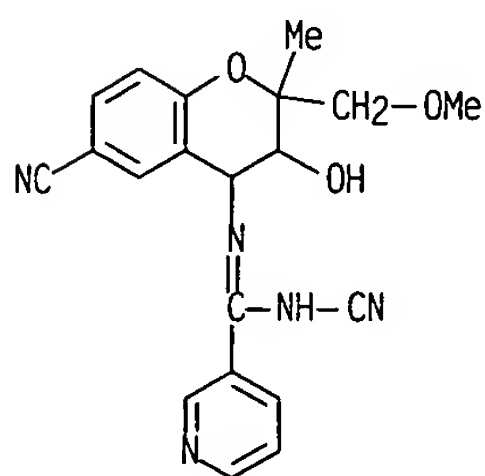
CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



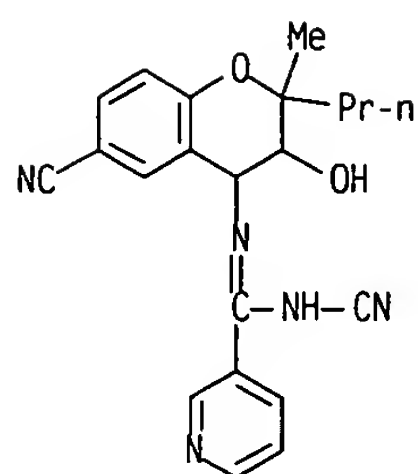
RN 180307-04-4 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]- (9CI) (CA INDEX NAME)



RN 180307-05-5 HCAPLUS

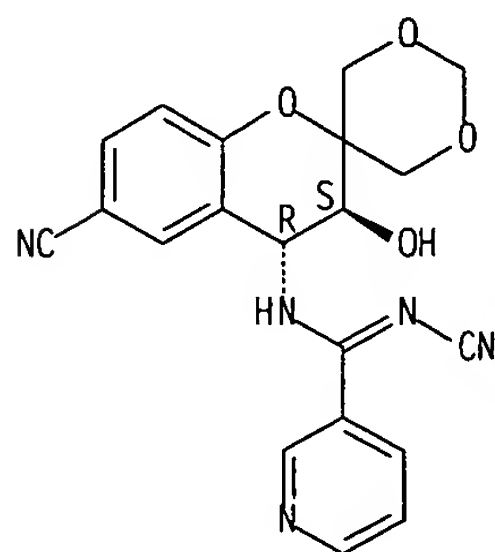
CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2-methyl-2-propyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 180470-15-9 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxyspiro[2H-1-benzopyran-2.5'-[1,3]dioxan]-4-yl)-, (3S-trans)- (9CI)
(CA INDEX NAME)

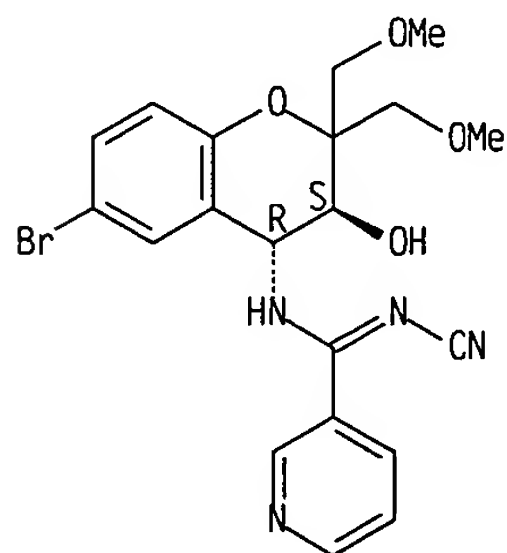
Absolute stereochemistry.
Double bond geometry unknown.



RN 180470-17-1 HCAPLUS

CN 3-Pyridinecarboximidamide, N-[6-bromo-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-N'-cyano-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L24 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:849162 HCAPLUS

DN 123:285779

ED Entered STN: 12 Oct 1995

TI Preparation of chroman derivs. as coronary vasodilators

IN Kato, Susumu; Cho, Hidetsura; Sayama, Shinsuke; Kajimoto, Yasuyuki;

Shibata, Saizo; Mizushima, Atsushi; Yamaki, Tokuo; Uchida, Itsuo
 PA Japan Tobacco Inc., Japan
 SO PCT Int. Appl.. 99 pp.
 CODEN: PIXXD2
 DT Patent
 LA Japanese
 IC ICM C07D311-68
 ICS C07D311-58; C07D405-12; C07D407-12; C07D409-12; C07D413-12;
 C07D417-12; C07D493-04; A61K031-35; C07F007-18
 CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 FAN.CNT 1

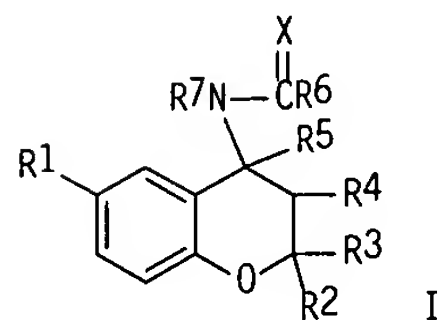
| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------|------|----------|-----------------|--------------|
| WO 9502589 | A1 | 19950126 | WO 1993-JP992 | 19930716 <-- |

W: CA, JP, KR, US
 RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE
 PRAI WO 1993-JP992 19930716 <--

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|--|
| WO 9502589 | ICM | C07D311-68 |
| | ICS | C07D311-58; C07D405-12; C07D407-12; C07D409-12; C07D413-12; C07D417-12; C07D493-04; A61K031-35; C07F007-18 |

OS MARPAT 123:285779
 GI



AB Chroman derivs. I (R1 = cyano, nitro, halogen; R2 = alkoxyalkyl, alkoxy carbonyl, hydroxyalkyl, aryloxyalkyl, tert-butyl dimethylsilyloxyalkyl; R3 = H, alkyl, alkoxyalkyl, alkoxy carbonyl, hydroxyalkyl, etc.; R4 = H, OH, formyloxy, alkanoyloxy; R5 = H; R4R5 may form bond; R6 = substituted aryl, heteroaryl, arylamino, aryloxy, alkyl; X = N-CN, O, S; R7 = H, lower alkyl), useful as coronary vasodilators, were prepared. Thus, stirring Et N-cyano-3-fluorobenzimidate with (3S,4R)-4-amino-6-cyano-3,4-dihydro-2,2-di(methoxymethyl)-3-hydroxy-2H-1-benzopyran in MeOH at room temperature for 1 day gave N'-cyano-N-[(3S,4R)-6-cyano-3,4-dihydro-2,2-di(methoxymethyl)-3-hydroxy-2H-1-benzopyran-4-yl]-3-fluorobenzimidine (II). II at 30 .mu.g/kg i.v. in dogs increased coronary blood flow with little blood pressure lowering effect.

ST chroman prepn coronary vasodilator
 IT Vasodilators
 (coronary, preparation of chroman derivs. as coronary vasodilators)

IT **168819-47-4P**
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of chroman derivs. as coronary vasodilators)

IT 98-88-4, Benzoyl chloride 103-71-9, reactions 621-87-4, 2-Propanone, 1-phenoxy- 1450-75-5 1450-76-6 1558-82-3, Ethanimidic acid, N-cyano-, ethyl ester 5271-67-0, Thenoyl chloride 5460-70-8,

2-Propanone,1,3-diethoxy- 18664-32-9 20260-53-1, 3-Pyridinecarbonyl
chloride, hydrochloride 33490-49-2 35794-84-4, Benzonitrile.
3-acetyl-4-hydroxy- 41835-08-9 79463-77-7 107326-06-7 133300-43-3
133300-49-9 134112-92-8 134113-09-0 149279-00-5, Benzenecarboximidic
acid, N-cyano-4-fluoro-, methyl ester 149279-01-6, 3-
Pyridinecarboximidic acid, N-cyano-, methyl ester 149279-07-2
149279-08-3 168819-01-0 168819-22-5 168819-49-6 168819-61-2
168819-83-8 169102-74-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of chroman derivs. as coronary vasodilators)

IT 168819-02-1P 168819-03-2P 168819-04-3P 168819-05-4P 168819-06-5P
168819-11-2P 168819-12-3P 168819-13-4P 168819-14-5P 168819-15-6P
168819-17-8P 168819-18-9P 168819-19-0P 168819-20-3P 168819-21-4P
168819-25-8P 168819-26-9P 168819-27-0P 168819-28-1P 168819-29-2P
168819-31-6P 168819-32-7P 168819-34-9P 168819-35-0P 168819-62-3P
168819-63-4P 168819-65-6P 168819-66-7P 168819-67-8P 168819-68-9P
168819-69-0P 168819-71-4P 168819-72-5P 168819-75-8P 168819-76-9P
168819-77-0P 168819-78-1P 168819-79-2P 169102-75-4P 169102-76-5P
169102-77-6P 169102-78-7P 169102-79-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation of chroman derivs. as coronary vasodilators)

IT 168819-33-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of chroman derivs. as coronary vasodilators)

IT 168819-07-6P 168819-08-7P 168819-09-8P
168819-10-1P 168819-16-7P 168819-23-6P
168819-24-7P 168819-30-5P 168819-36-1P
168819-37-2P 168819-38-3P 168819-39-4P
168819-40-7P 168819-41-8P 168819-42-9P
168819-43-0P 168819-44-1P 168819-45-2P
168819-46-3P 168819-48-5P 168819-50-9P
168819-51-0P 168819-52-1P 168819-53-2P 168819-54-3P 168819-55-4P
168819-56-5P 168819-57-6P 168819-58-7P 168819-59-8P
168819-60-1P 168819-64-5P 168819-70-3P
168819-73-6P 168819-74-7P 168819-80-5P
168819-81-6P 168819-82-7P 169273-22-7P
169273-23-8P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological
study); PREP (Preparation); USES (Uses)

(preparation of chroman derivs. as coronary vasodilators)

IT 168819-47-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)

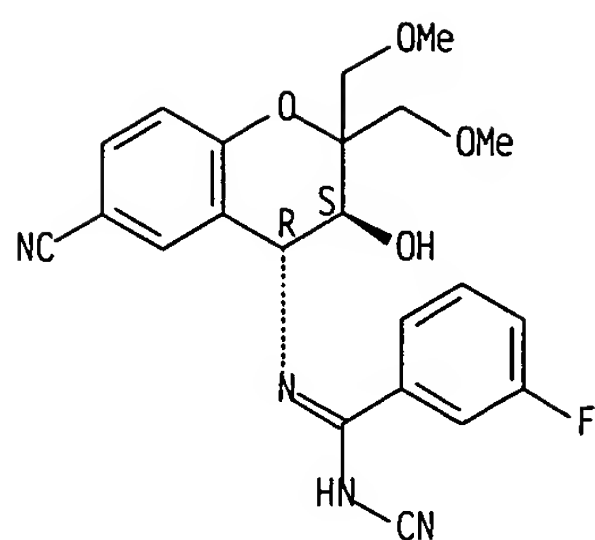
(preparation of chroman derivs. as coronary vasodilators)

RN 168819-47-4 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-
bis(methoxymethyl)-2H-1-benzopyran-4-yl]-3-fluoro-, (3S-trans)- (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.



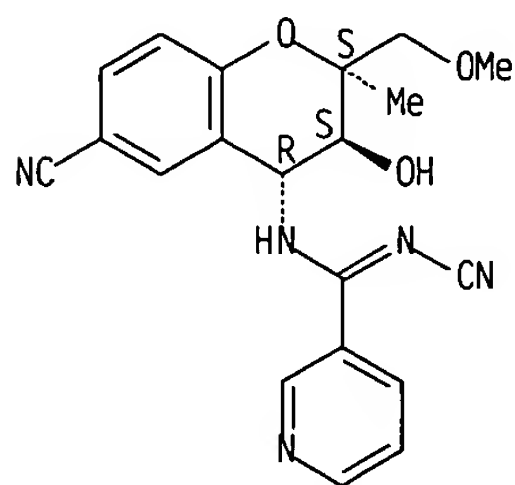
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 168819-24-7P 168819-30-5P 168819-36-1P
 168819-37-2P 168819-38-3P 168819-39-4P
 168819-40-7P 168819-41-8P 168819-42-9P
 168819-43-0P 168819-44-1P 168819-45-2P
 168819-46-3P 168819-48-5P 168819-50-9P
 168819-58-7P 168819-64-5P 168819-70-3P
 168819-73-6P 168819-74-7P 168819-80-5P
 168819-81-6P 168819-82-7P 169273-22-7P
 169273-23-8P

RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of chroman derivs. as coronary vasodilators)

RN 168819-07-6 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]-, (2.alpha.,3.alpha.,4.beta.)- (9CI) (CA INDEX NAME)

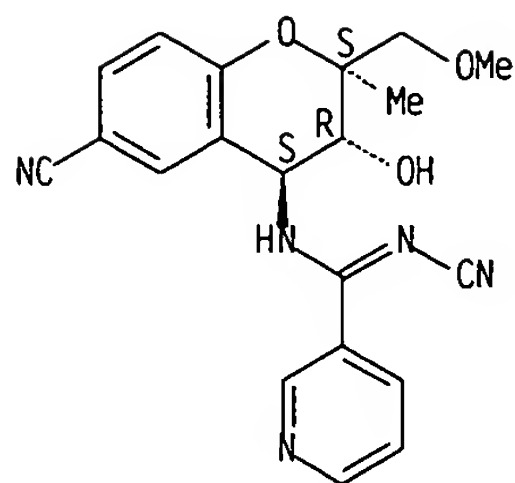
Relative stereochemistry.
 Double bond geometry unknown.



RN 168819-08-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]-, (2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)

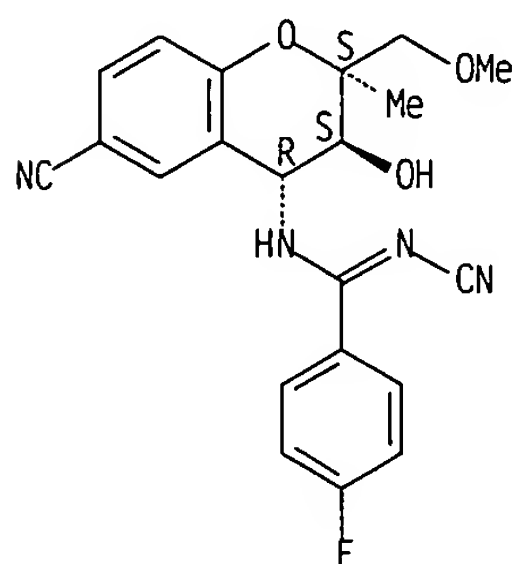
Relative stereochemistry.
 Double bond geometry unknown.



RN 168819-09-8 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]-4-fluoro-, (2.alpha.,3.alpha.,4.beta.)- (9CI) (CA INDEX NAME)

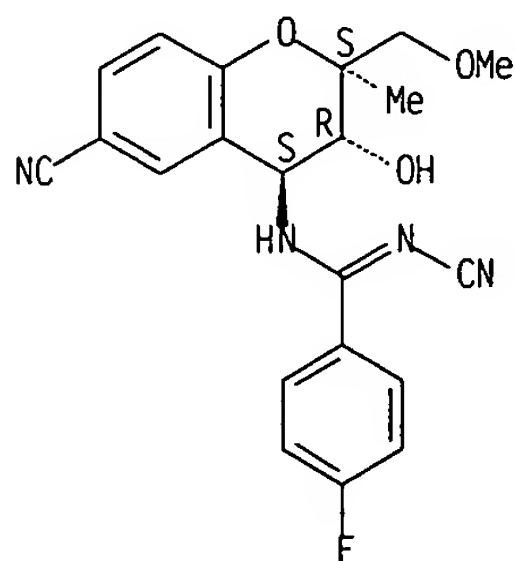
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-10-1 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]-4-fluoro-, (2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)

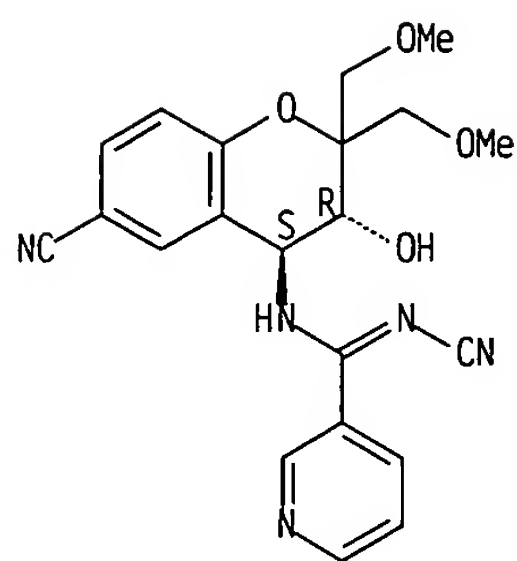
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-16-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

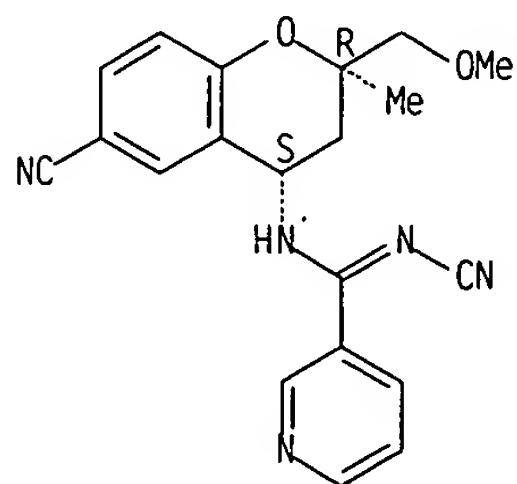
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-23-6 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

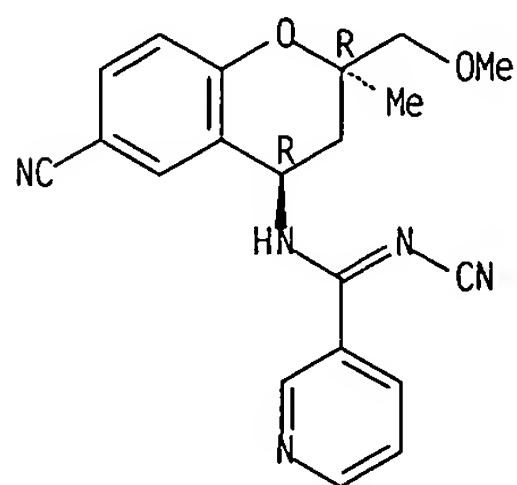
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-24-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2-(methoxymethyl)-2-methyl-2H-1-benzopyran-4-yl]-, cis- (9CI) (CA INDEX NAME)

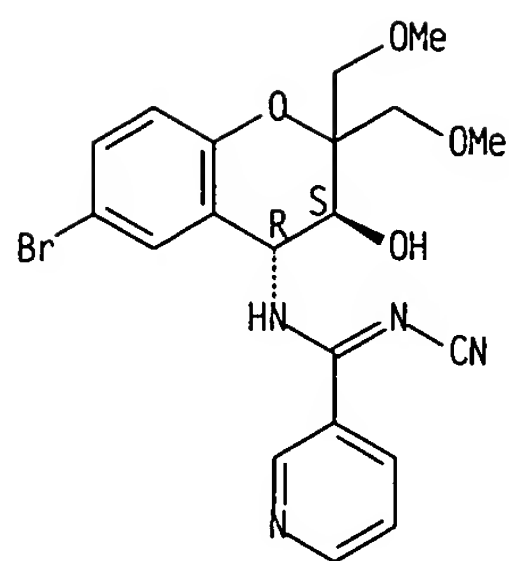
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-30-5 HCAPLUS

CN 3-Pyridinecarboximidamide, N-[6-bromo-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-N'-cyano-, trans- (9CI) (CA INDEX NAME)

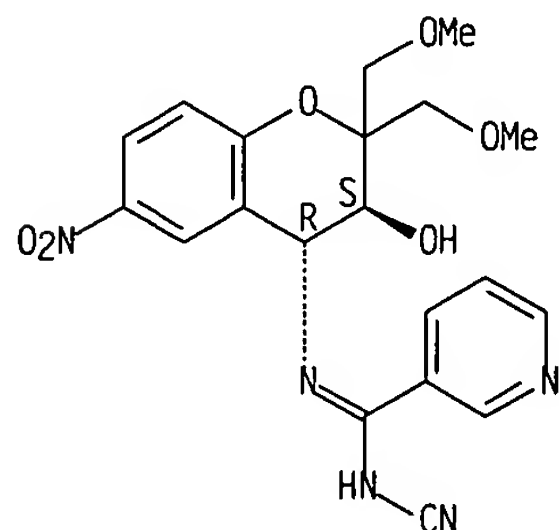
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-36-1 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

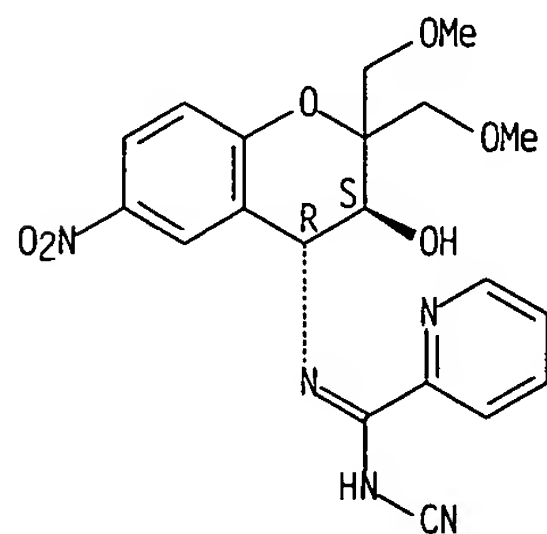
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-37-2 HCAPLUS

CN 2-Pyridinecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

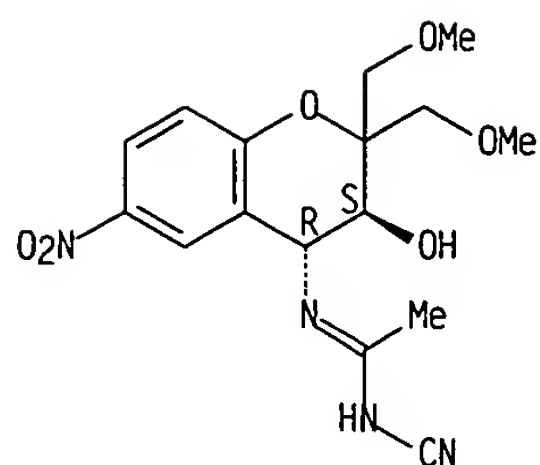
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-38-3 HCAPLUS

CN Ethanimidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

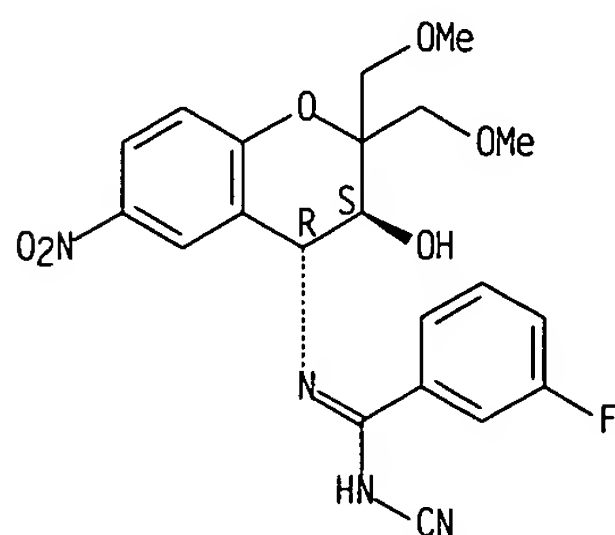
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-39-4 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-3-fluoro-, (3S-trans)- (9CI) (CA INDEX NAME)

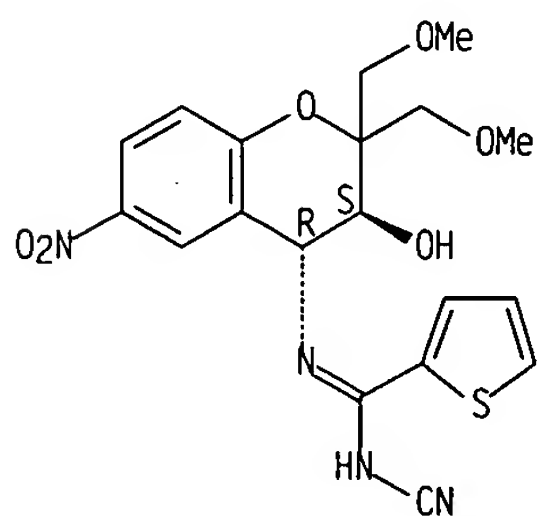
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-40-7 HCAPLUS

CN 2-Thiophenecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

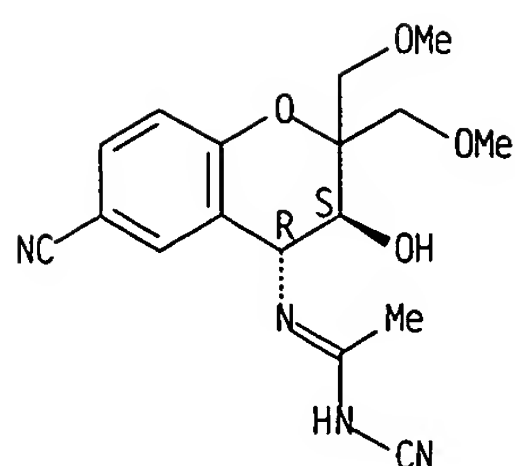
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-41-8 HCAPLUS

CN Ethanimidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

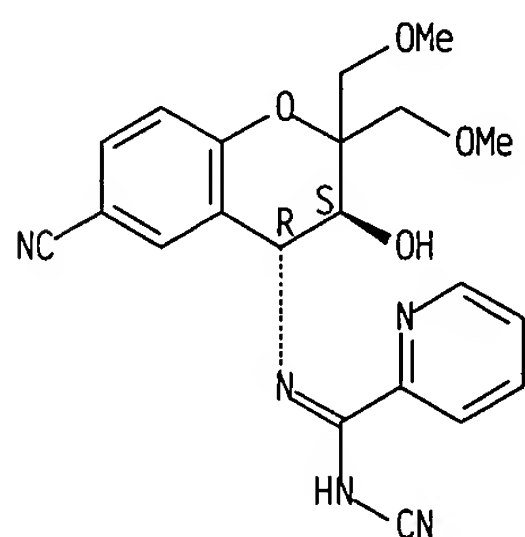
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-42-9 HCAPLUS

CN 2-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

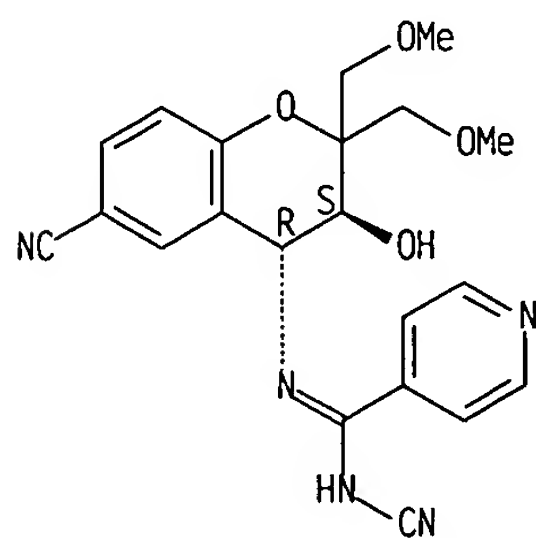
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-43-0 HCAPLUS

CN 4-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

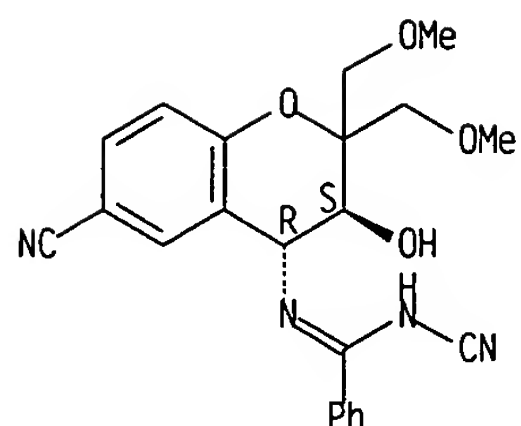
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-44-1 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

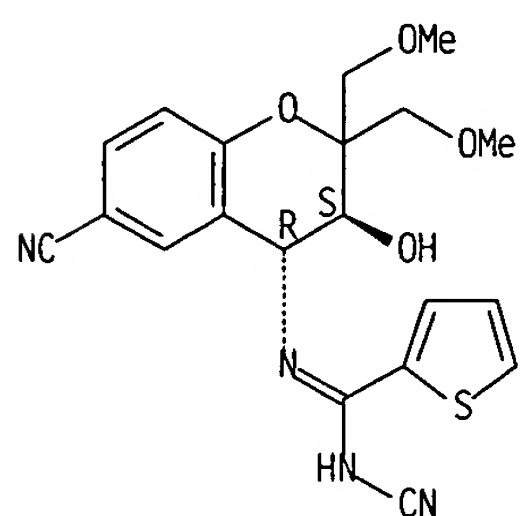
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-45-2 HCAPLUS

CN 2-Thiophenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

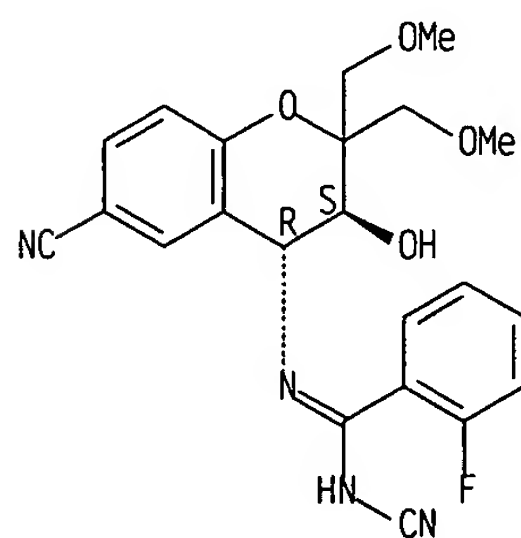
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-46-3 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-2-fluoro-, (3S-trans)- (9CI) (CA INDEX NAME)

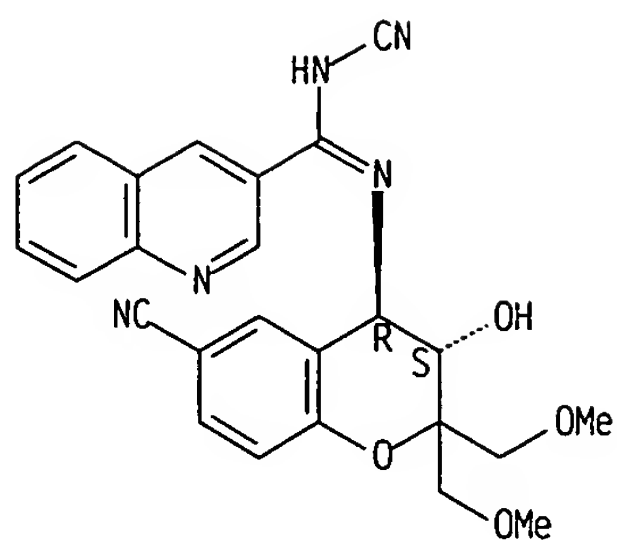
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-48-5 HCAPLUS

CN 3-Quinolinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

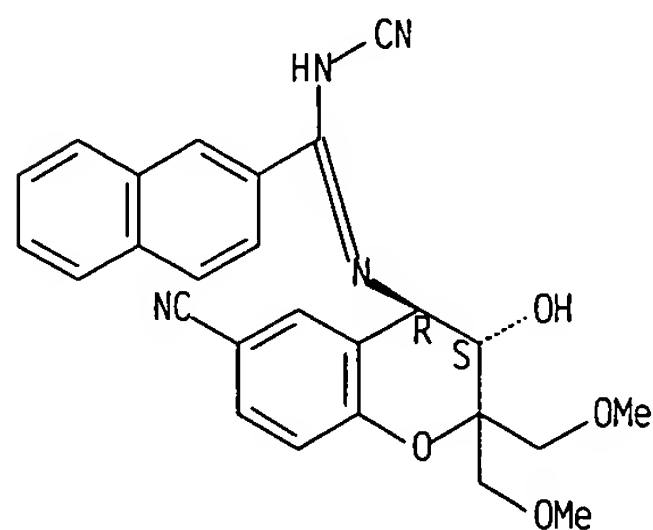
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-50-9 HCAPLUS

CN 2-Naphthalenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

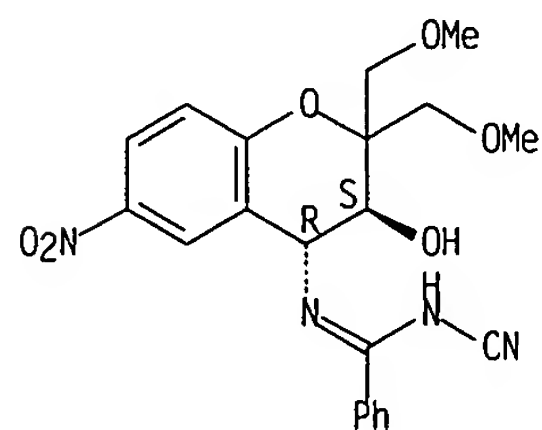
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-58-7 HCAPLUS

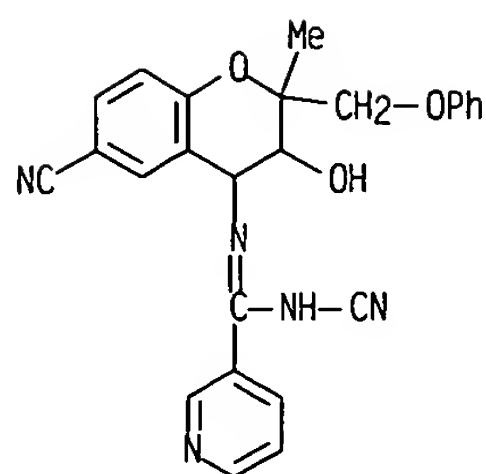
CN Benzenecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-6-nitro-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-64-5 HCAPLUS

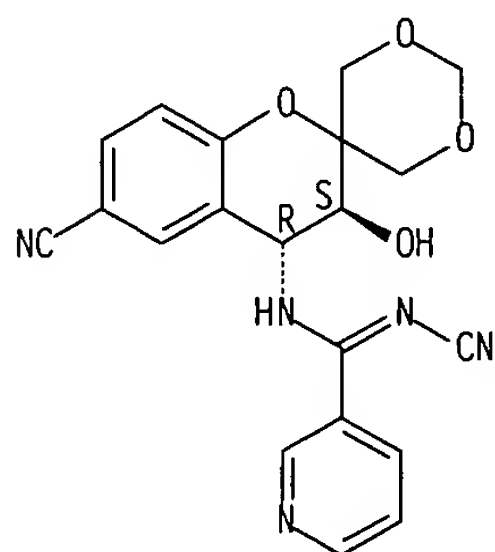
CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2-methyl-2-(phenoxymethyl)-2H-1-benzopyran-4-yl]- (9CI) (CA INDEX NAME)



RN 168819-70-3 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxyspiro[2H-1-benzopyran-2,5'-[1,3]dioxan]-4-yl)-, trans- (9CI) (CA INDEX NAME)

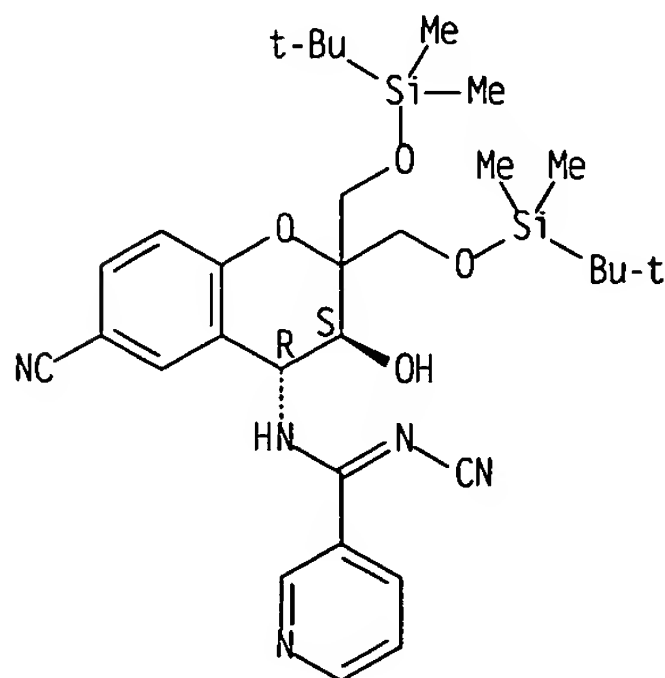
Relative stereochemistry.
Double bond geometry unknown.



RN 168819-73-6 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-2,2-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-3,4-dihydro-3-hydroxy-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

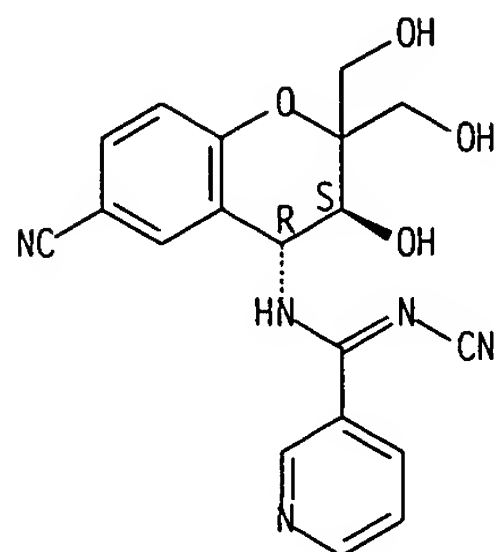


RN 168819-74-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(hydroxymethyl)-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

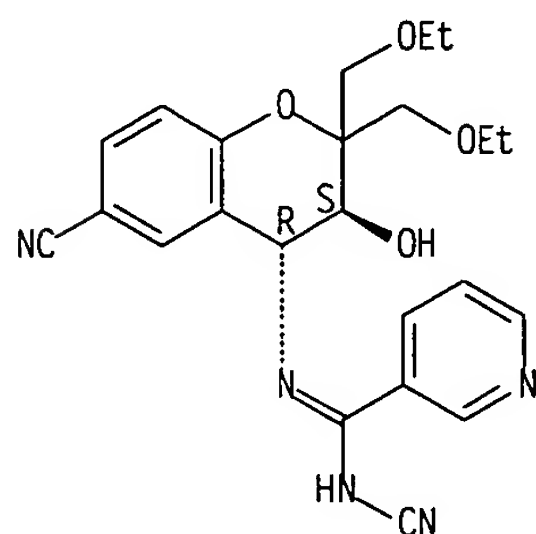
Double bond geometry unknown.



RN 168819-80-5 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-2,2-bis(ethoxymethyl)-3,4-dihydro-3-hydroxy-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

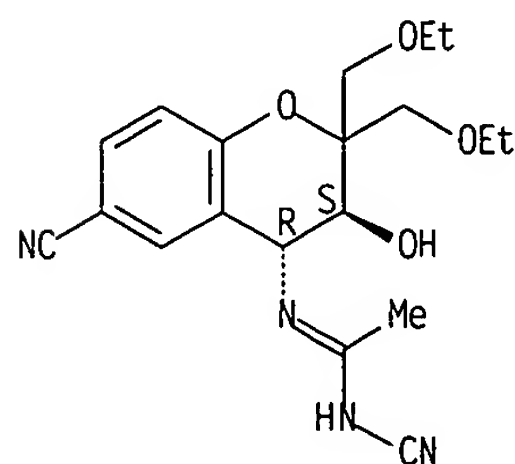
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-81-6 HCAPLUS

CN Ethanamide, N-cyano-N'-[6-cyano-2,2-bis(ethoxymethyl)-3,4-dihydro-3-hydroxy-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

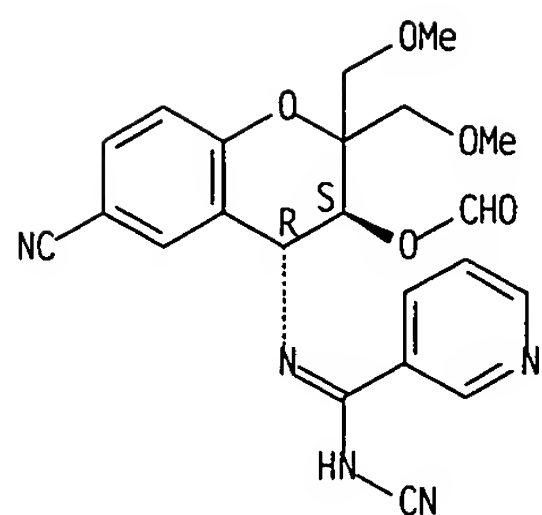
Absolute stereochemistry.
Double bond geometry unknown.



RN 168819-82-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3-(formyloxy)-3,4-dihydro-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

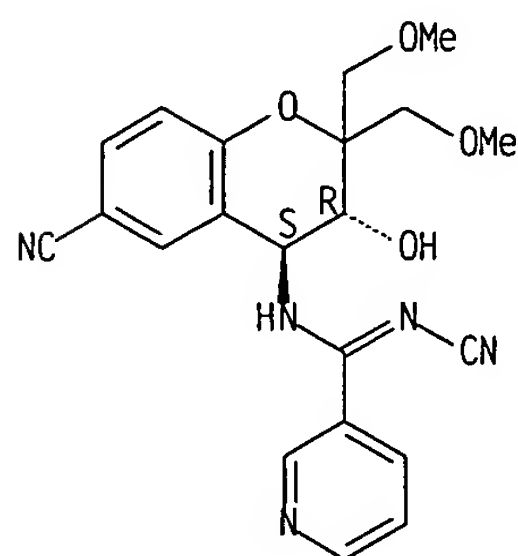
Absolute stereochemistry.
Double bond geometry unknown.



RN 169273-22-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3R-trans)- (9CI) (CA INDEX NAME)

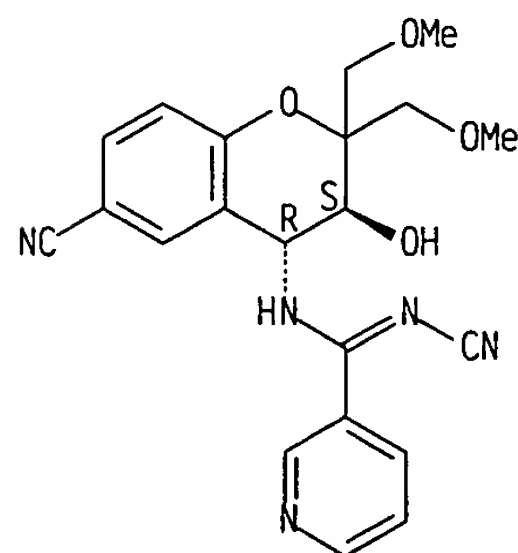
Absolute stereochemistry.
Double bond geometry unknown.



RN 169273-23-8 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-3-hydroxy-2,2-bis(methoxymethyl)-2H-1-benzopyran-4-yl]-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L24 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:339492 HCAPLUS

DN 122:105674

ED Entered STN: 08 Feb 1995

TI Preparation of 4-[[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivatives as antihypertensive agents and vasodilators

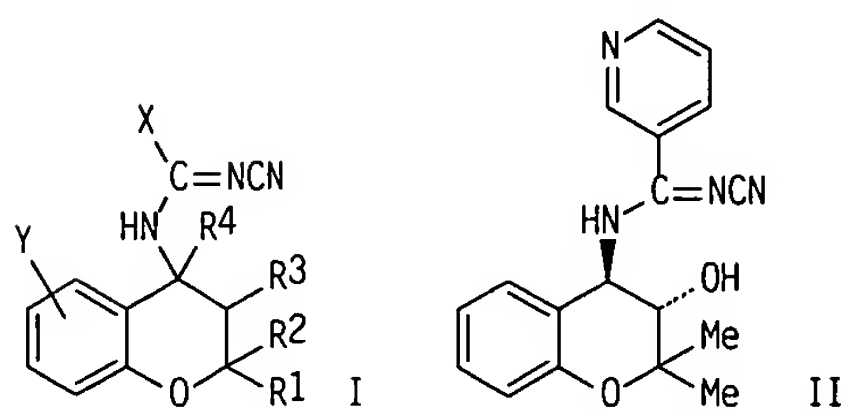
IN Nakajima, Tatsuo; Sakai, Teruyuki; Izawa, Toshio
 PA Kirin Brewery, Japan
 SO Jpn. Kokai Tokkyo Koho, 9 pp.
 CODEN: JKXXAF
 DT Patent
 LA Japanese
 IC ICM C07D405-12
 ICS A61K031-35; A61K031-38; A61K031-44; C07D407-12; C07D409-12
 CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 FAN.CNT 1

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|---------------|------|----------|-----------------|--------------|
| JP 06298759 | A2 | 19941025 | JP 1993-93363 | 19930420 <-- |
| JP 1993-93363 | | 19930420 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|-------------|-------|--|
| JP 06298759 | ICM | C07D405-12 |
| | ICS | A61K031-35; A61K031-38; A61K031-44; C07D407-12; C07D409-12 |

OS MARPAT 122:105674
 GI



AB The title compds. [I; X = (un)substituted heteroaryl; Y = cyano, NO₂, CF₃, MeSO₂; R₁, R₂ = lower alkyl; R₃ = OZ, wherein Z = H, acyl, alkylsulfonyl, or arylsulfonyl; R₄ = H or R₄R₃ forms a bond], having potent and long-lasting antihypertensive activity due to the activation of K⁺ channel, are prepared. Thus, 3-cyanopyridine was treated with HCl(g) in propanol at 0-5.degree. to give crude Pr 3-pyridinecarboximide which was cyanated with cyanamide in aqueous solution of NaH₂PO₄.2H₂O and Na₂HPO₄ to give Pr N-cyano-3-pyridinecarboximide. The latter compound was condensed with (+)-(3S,4R)-trans-4-amino-3,4-dihydro-2,2-dimethyl-3-hydroxy-2H-1-benzopyran-6-carbonitrile in MeOH to give title compound [(-)-(3S,4R)-trans-II]. II showed ED₅₀ of 30.2 mg/kg peritoneally for reducing the blood pressure of spontaneously hypertensive rats and the hypertensive effect lasted for .gtoreq.24 h.

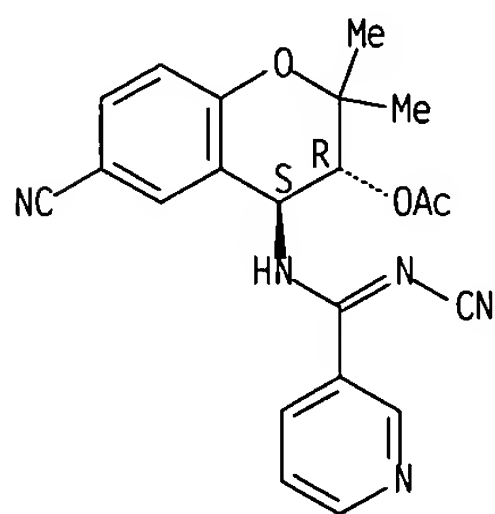
ST heterocyclylcianoiminomethylaminobenzopyran prepn antihypertensive; vasodilator heterocyclylcianoiminomethylaminobenzopyran; aminobenzopyran heterocyclylcianoiminomethyl prepn antihypertensive; cyanoiminomethylaminobenzopyran heterocyclyl prepn antihypertensive

IT Antihypertensives
 Vasodilators
 (preparation of [[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivs. as antihypertensive agents and vasodilators)

IT 143966-29-4P 143966-30-7P. 3-Pyridinecarboximidic acid, N-cyano, propyl ester 149278-54-6P 160753-73-1P 160753-74-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

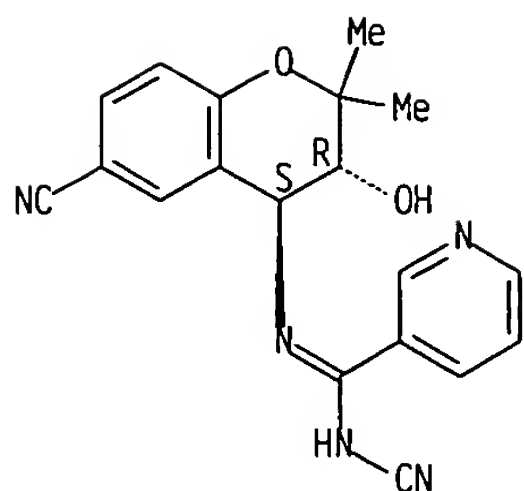
- (intermediate for preparation of [[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivs. as antihypertensive agents and vasodilators)
- IT 149278-33-1P 149278-68-2P 149342-19-8P
160753-70-8P 160753-71-9P 160753-72-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivs. as antihypertensive agents and vasodilators)
- IT 100-54-9, 3-Cyanopyridine 108-24-7, Acetic anhydride 420-04-2, Cyanamide 86776-58-1 88653-55-8 102423-21-2, Methyl N-cyano-2-furancarboximidate 118581-55-8 133300-52-4, Methyl N-cyano-3-thiophenecarboximidate
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction in preparation of [[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivs. as antihypertensive agents and vasodilators)
- IT 149278-54-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate for preparation of [[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivs. as antihypertensive agents and vasodilators)
- RN 149278-54-6 HCAPLUS
- CN 3-Pyridinecarboximidamide, N-[3-(acetyloxy)-6-cyano-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-N'-cyano-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



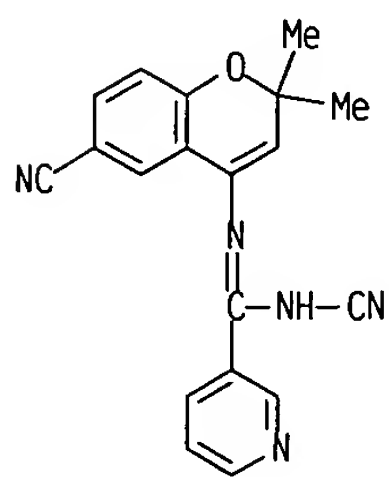
- IT 149278-33-1P 149278-68-2P 149342-19-8P
160753-70-8P 160753-71-9P 160753-72-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of [[heterocyclyl(cyanoimino)methyl]amino]benzopyran derivs. as antihypertensive agents and vasodilators)
- RN 149278-33-1 HCAPLUS
- CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RN 149278-68-2 HCAPLUS

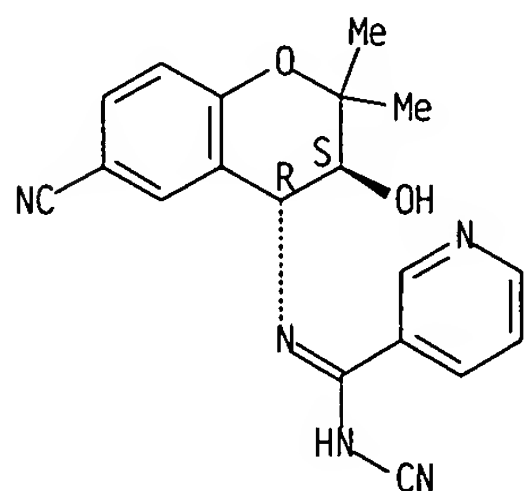
CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 149342-19-8 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, (3S-trans)- (9CI) (CA INDEX NAME)

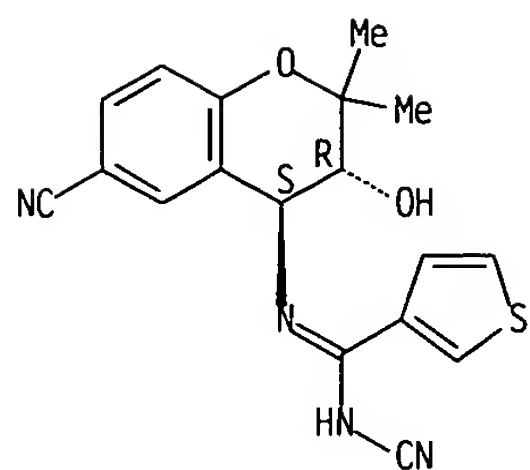
Absolute stereochemistry.
Double bond geometry unknown.



RN 160753-70-8 HCAPLUS

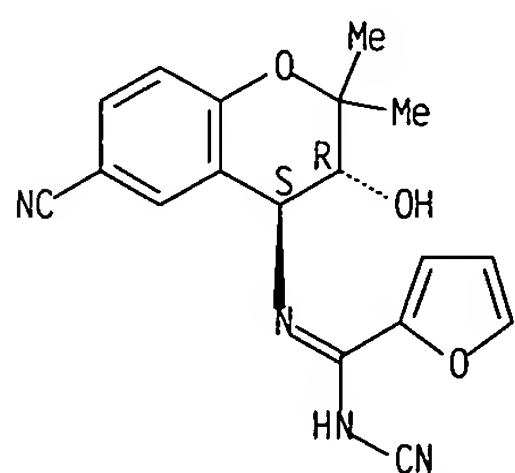
CN 3-Thiophenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



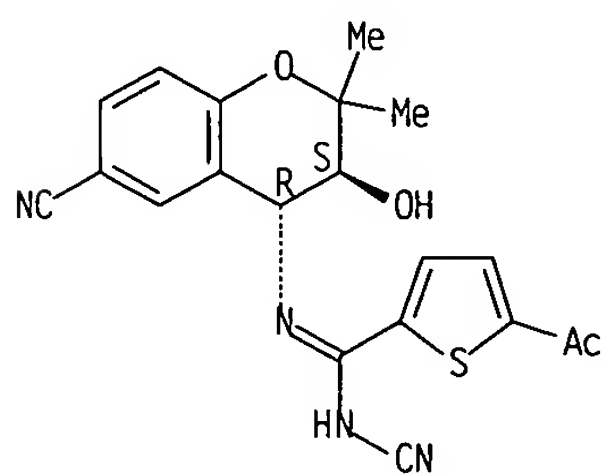
RN 160753-71-9 HCAPLUS
 CN 2-Furancarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



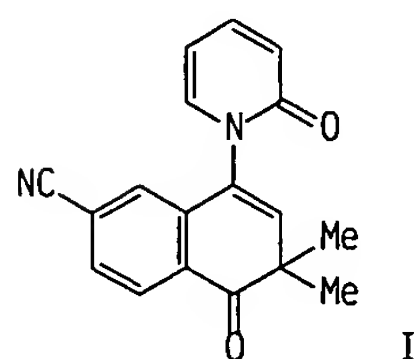
RN 160753-72-0 HCAPLUS
 CN 2-Thiophenecarboximidamide, 5-acetyl-N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, (3S-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



L24 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1993:560066 HCAPLUS
 DN 119:160066
 ED Entered STN: 16 Oct 1993
 TI 2,2-Dialkyl-naphthalen-1-ones as new potassium channel activators
 AU Almansa, Carmen; Gomez, Luis A.; Cavalcanti, Fernando L.; Rodriguez, Ricardo; Carceller, Elena; Bartroli, Javier; Garcia-Rafanell, Julian; Forn, Javier
 CS Res. Cent., J. Uriach y Cia.S.A., Barcelona, 08026, Spain
 SO Journal of Medicinal Chemistry (1993), 36(15), 2121-33
 CODEN: JMCMAR; ISSN: 0022-2623

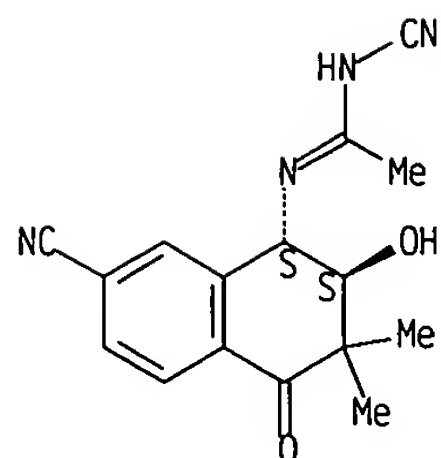
DT Journal
 LA English
 CC 27-17 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1, 25
 GI



- AB A new series of 2,2-dialkyl-naphthalen-1-one potassium channel activators has been prepared, and their in vitro relaxant activities in isolated rat portal vein and guinea pig tracheal spirals as well as their oral antihypertensive effect in spontaneously hypertensive rats have been evaluated. The group of 1,2-dihydro-4-(1,2-dihydro-2-oxo-1-pyridyl)-2,2-dimethylnaphthalen-1-ones with an electron-withdrawing substituent at the 6-position contain the most active compds. and 1,2-dihydro-4-(1,2-dihydro-2-oxo-1-pyridyl)-2,2-dimethyl-1-oxonaphthalene-6-carbonitrile, (UR-8225) (I), has been selected for further pharmacol. development.
- ST dialkyl-naphthalenone prepn potassium channel activator; naphthalenone dialkyl prepn potassium channel activator; antihypertensive dialkyl-naphthalenone prepn; structure activity relationship dialkyl-naphthalenone antihypertensive
- IT Antihypertensives
 Bronchodilators
 (dialkyl-naphthalenones)
- IT Molecular structure-biological activity relationship
 (antihypertensive, of dialkyl-naphthalenones)
- IT Ion channel openers
 (potassium, dialkyl-naphthalenones)
- IT 4635-59-0, 4-Chlorobutyryl chloride
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (cyclocondensation of, with aminotetrahydronaphthalenone derivative)
- IT 703-67-3 1078-19-9 25095-57-2 26673-31-4 32281-97-3 62620-71-7
 66361-67-9 90401-84-6 149456-02-0 149915-80-0 149915-81-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (methylation of)
- IT 149456-22-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and bromination of)
- IT 149455-39-0P 149455-77-6P 149455-81-2P 149455-86-7P 149455-90-3P
 149455-94-7P 149455-99-2P 149456-05-3P 149456-10-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclization of, with chlorobutyryl chloride)
- IT 21568-65-0P 148925-37-5P 149455-83-4P 149455-88-9P 149455-92-5P
 149455-96-9P 149456-01-9P 149456-07-5P 149456-12-2P 149456-15-5P
 149456-18-8P 149456-23-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and dehydrogenation of)
- IT 148925-38-6P 149455-79-8P 149455-84-5P 149455-89-0P 149455-93-6P
 149455-97-0P 149456-03-1P 149456-08-6P 149456-13-3P 149456-16-6P
 149456-19-9P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

(Reactant or reagent)
 (preparation and epoxidn. of)
 IT 149915-77-5P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and hydrolysis of)
 IT 149455-91-4P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and intramol. cyclization of)
 IT 155267-76-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and methylation or acetylation of)
 IT 94535-50-9P 148925-41-1P 148925-42-2P 148925-46-6P 148925-49-9P
 148925-52-4P 148925-53-5P 148925-54-6P 148925-55-7P 148925-60-4P
 148925-61-5P 148925-62-6P 148925-64-8P **148925-65-9P**
 149455-11-8P 149455-13-0P 149455-15-2P 149455-16-3P 149455-18-5P
 149455-19-6P 149455-21-0P 149455-23-2P 149455-24-3P 149455-25-4P
 149455-26-5P 149455-28-7P 149455-31-2P 149455-32-3P 149455-33-4P
 149455-34-5P 149455-35-6P 149455-36-7P 149455-38-9P 149455-40-3P
 149455-41-4P 149455-42-5P 149455-43-6P 149455-44-7P 149455-46-9P
 149455-48-1P 149455-50-5P 149455-51-6P 149455-52-7P 149455-53-8P
 149455-54-9P 149455-55-0P 149455-56-1P 149455-57-2P 149455-59-4P
 149455-60-7P 149455-61-8P 149455-62-9P 149455-64-1P 149455-65-2P
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 155267-81-5P 155267-82-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and potassium channel activator activity of)
 IT 148925-39-7P 148925-40-0P 148925-50-2P 149455-76-5P 149455-80-1P
 149455-85-6P 149455-98-1P 149456-04-2P 149456-09-7P 149456-14-4P
 149456-17-7P 149456-20-2P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)
 (preparation and reaction of, with amines)
 IT 149455-30-1P 149915-78-6P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 IT 142-08-5, 2-Hydroxypyridine 18292-04-1
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with bromoepoxytetrahydronaphthalenone derivative)
 IT **148925-65-9P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and potassium channel activator activity of)
 RN 148925-65-9 HCAPLUS
 CN Ethanimidamide, N-cyano-N'-(7-cyano-1,2,3,4-tetrahydro-2-hydroxy-3,3-
 dimethyl-4-oxo-1-naphthalenyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



L24 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:539100 HCAPLUS

DN 119:139100

ED Entered STN: 02 Oct 1993

TI Preparation of benzopyran derivatives as antihypertensives and vasodilators.

IN Katoh, Susumu; Sayama, Shinsuke; Shibata, Saizo; Uchida, Itsuo

PA Japan Tobacco Inc., Japan

SO PCT Int. Appl., 91 pp.

CODEN: PIXXD2

DT Patent

LA Japanese

IC ICM C07D311-68

ICS C07D405-12; C07D409-12

ICA A61K031-35

ICI C07D405-12, C07D213-00, C07D311-00; C07D409-12, C07D311-00, C07D333-00

CC 27-14 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

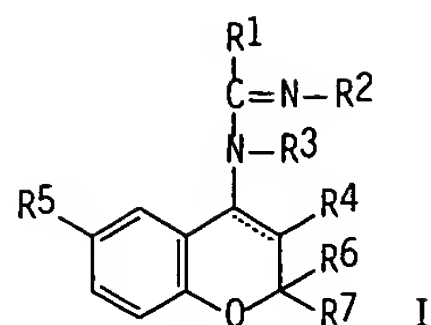
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|------|---|------|----------|-----------------|--------------|
| PI | WO 9219611 | A1 | 19921112 | WO 1992-JP538 | 19920424 <-- |
| | W: CA, HU, KR, RU, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE | | | | |
| | JP 05186458 | A2 | 19930727 | JP 1992-137484 | 19920415 <-- |
| | CA 2086322 | AA | 19921027 | CA 1992-2086322 | 19920424 <-- |
| | EP 536424 | A1 | 19930414 | EP 1992-909551 | 19920424 <-- |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, SE | | | | |
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| PRAI | JP 1991-188374 | A | 19910426 | <-- | |
| | JP 1991-279014 | A | 19910730 | <-- | |
| | JP 1992-137484 | A | 19920415 | <-- | |
| | WO 1992-JP538 | W | 19920424 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|--|
| WO 9219611 | ICM | C07D311-68 |
| | ICS | C07D405-12; C07D409-12 |
| | ICA | A61K031-35 |
| | ICI | C07D405-12, C07D213-00, C07D311-00; C07D409-12, C07D311-00, C07D333-00 |

OS MARPAT 119:139100

GI



AB The title compds. [I; R1 = halo, NO₂, alkoxycarbonyl, (un)substituted alkyl; R2 = OH, alkoxy, cyano, NO₂, etc.; R3 = H, alkyl; R4 = H, OH, nitrooxy, Ac; R5 = alkyl, (un)substituted alkoxy, cyano, NO₂, acyl, halo; R6, R7 = alkyl, or R6R7 = alkylene] and their pharmaceutically acceptable salts are prepared Me N-[trans-3-(tert-butyldimethylsilyloxy)-6-cyano-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-3-pyridinethiocarboximide (preparation given) in diglyme was treated with cyanamide at 80.degree. to give N-[trans-3-(tert-butyldimethylsilyloxy)-6-cyano-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-N'-cyano-3-pyridinethiocarboximide, which was treated with Bu₄NF at room temperature for 4 days to give I [R1 = 3-pyridyl, R2 = R5 = cyano, R3 = H, R4 = OH, R6 = R7 = Me], which had an IC₅₀ of 0.6 .mu.M as a vasodilator in an in vitro study.

ST benzopyran deriv prepn antihypertensive vasodilator; antihypertensive benzopyran deriv prepn

IT Antihypertensives
Vasodilators

(benzopyran derivs.)

IT 149278-31-9P 149278-32-0P **149278-33-1P** 149278-34-2P
149278-35-3P **149278-36-4P** 149278-37-5P 149278-38-6P
149278-39-7P **149278-40-0P** 149278-41-1P 149278-42-2P
149278-43-3P 149278-44-4P **149278-45-5P** **149278-46-6P**
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149342-21-2P **149342-22-3P**

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as antihypertensive and vasodilator)

IT 31084-70-5P 149278-71-7P 149278-72-8P 149278-73-9P 149278-74-0P
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149278-79-5P 149278-80-8P 149278-81-9P 149278-82-0P
149278-83-1P 149278-84-2P 149278-85-3P 149278-86-4P 149278-87-5P
149278-88-6P 149278-89-7P 149278-90-0P 149278-91-1P
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149278-97-7P 149278-98-8P 149857-13-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for antihypertensives and vasodilators)

IT 67-62-9, O-Methylhydroxylamine 74-88-4, Methyl iodide, reactions
108-48-5, 2,6-Lutidine 420-04-2, Cyanamide 541-41-3, Ethyl
chloroformate 831-68-5, Ethyl 4-nitrobenzimidate 7803-49-8,
Hydroxylamine, reactions 10400-19-8, 3-Pyridinecarbonyl chloride
18162-48-6, tert-Butyldimethylsilyl chloride 19547-38-7, Methyl
2-pyridinecarboximide 19847-10-0, Pyrazinecarbonyl chloride
52162-47-7 86776-58-1 86823-96-3 89316-86-9 95460-34-7
99498-54-1 107326-06-7, Methyl N-cyano-2-thiophenecarboximide
118581-55-8 121021-87-2 124787-48-0 127419-05-0 129462-75-5
133178-68-4 133300-43-3 133415-43-7 149278-99-9 149279-00-5
149279-01-6 149279-02-7 149279-03-8 149279-04-9 149279-05-0
149279-06-1 149279-07-2 149279-08-3 149279-09-4 149279-10-7

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of antihypertensives and vasodilators)

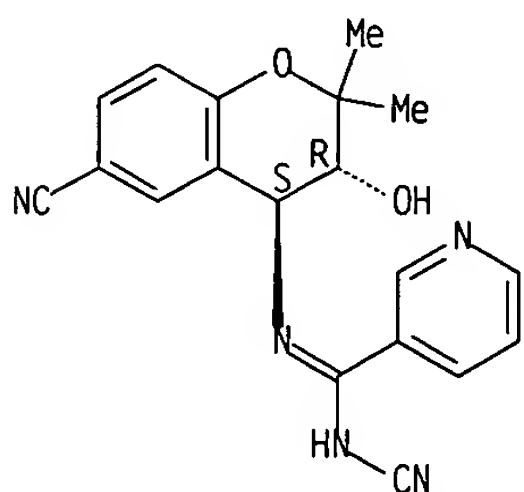
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 149278-62-6P 149278-63-7P 149278-64-8P
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 149278-68-2P 149278-69-3P 149278-70-6P
 149342-19-8P 149342-20-1P 149342-21-2P
 149342-22-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as antihypertensive and vasodilator)

RN 149278-33-1 HCAPLUS

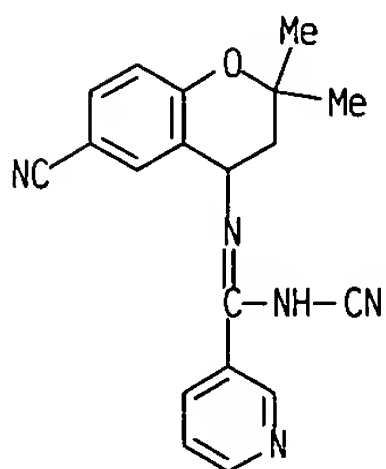
CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



RN 149278-36-4 HCAPLUS

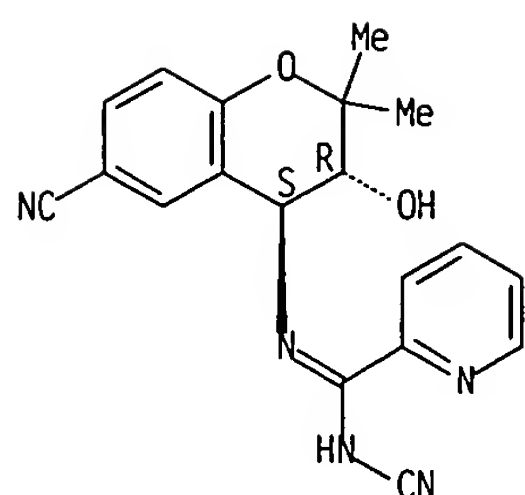
CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 149278-39-7 HCAPLUS

CN 2-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

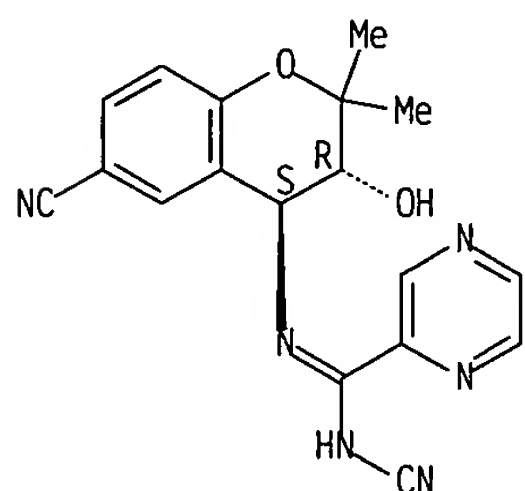
Relative stereochemistry.
 Double bond geometry unknown.



RN 149278-40-0 HCAPLUS

CN Pyrazinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

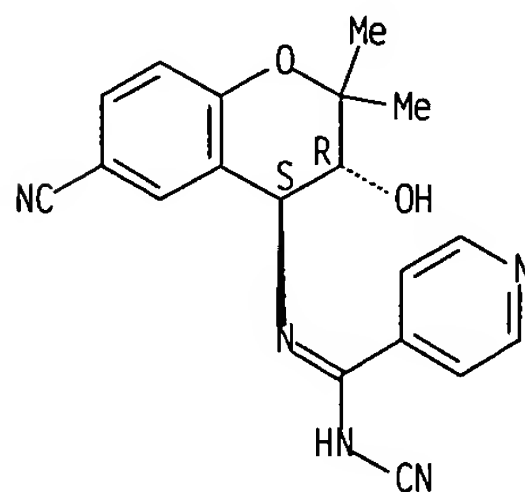
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-45-5 HCAPLUS

CN 4-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

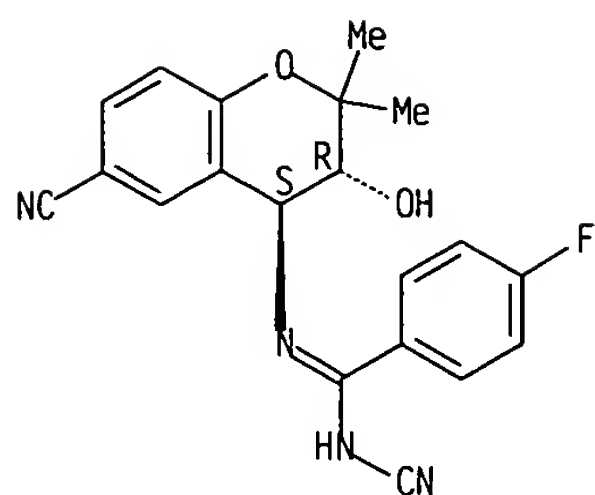
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-46-6 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-fluoro-, trans- (9CI) (CA INDEX NAME)

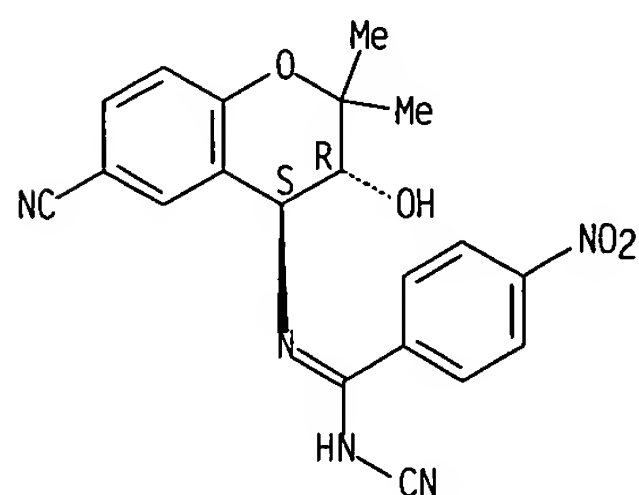
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-51-3 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-nitro-, trans- (9CI) (CA INDEX NAME)

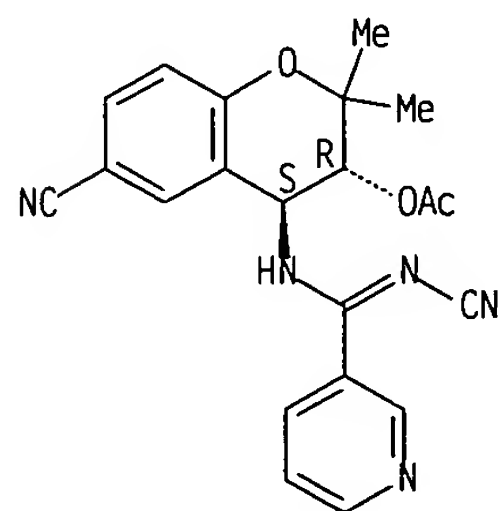
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-54-6 HCAPLUS

CN 3-Pyridinecarboximidamide, N-[3-(acetyloxy)-6-cyano-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-N'-cyano-, trans- (9CI) (CA INDEX NAME)

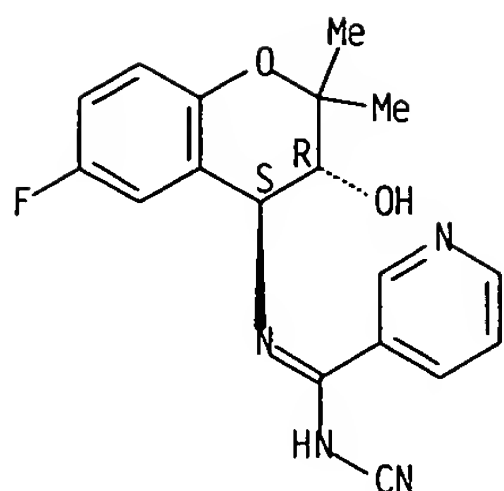
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-55-7 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-fluoro-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

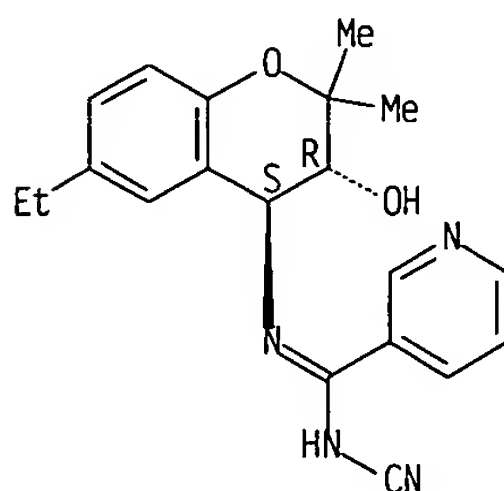
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-56-8 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-ethyl-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

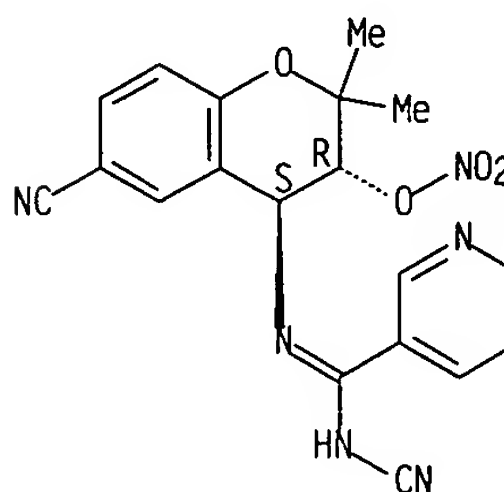
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-57-9 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2,2-dimethyl-3-(nitrooxy)-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

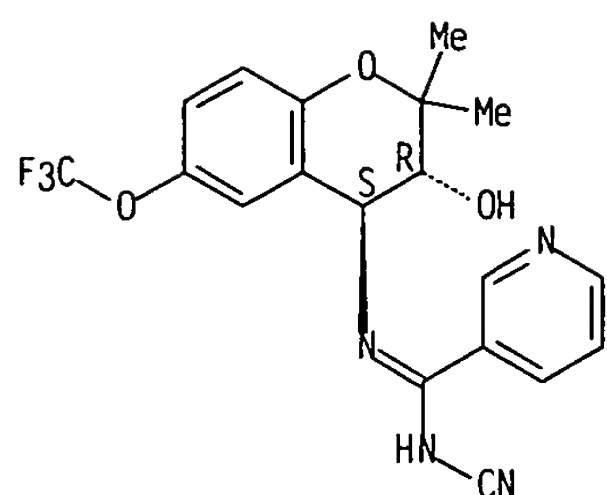
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-58-0 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-dimethyl-6-(trifluoromethoxy)-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

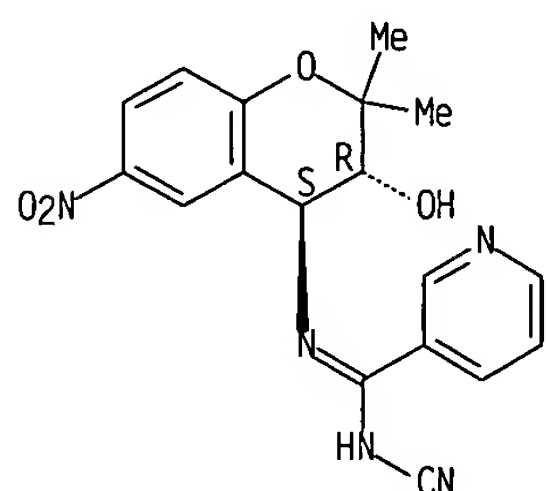
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-59-1 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

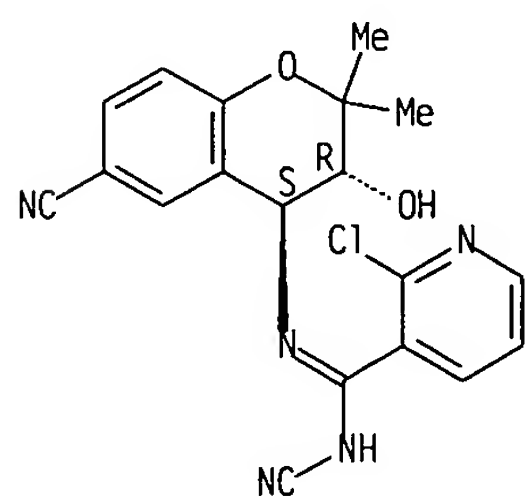
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-60-4 HCAPLUS

CN 3-Pyridinecarboximidamide, 2-chloro-N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

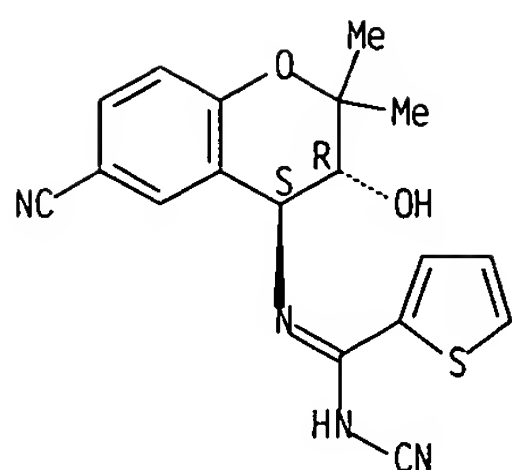
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-61-5 HCAPLUS

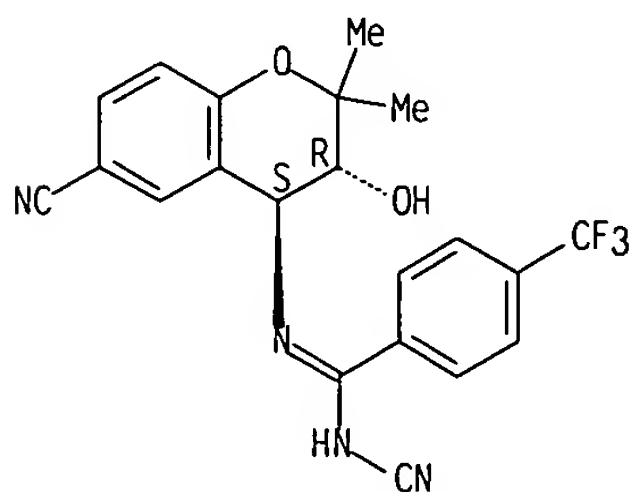
CN 2-Thiophenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



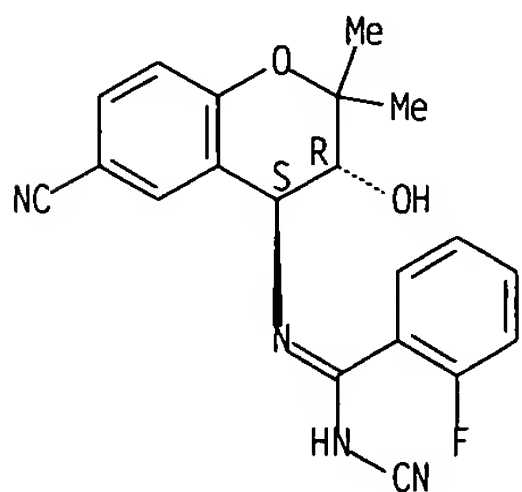
RN 149278-62-6 HCAPLUS
 CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-(trifluoromethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



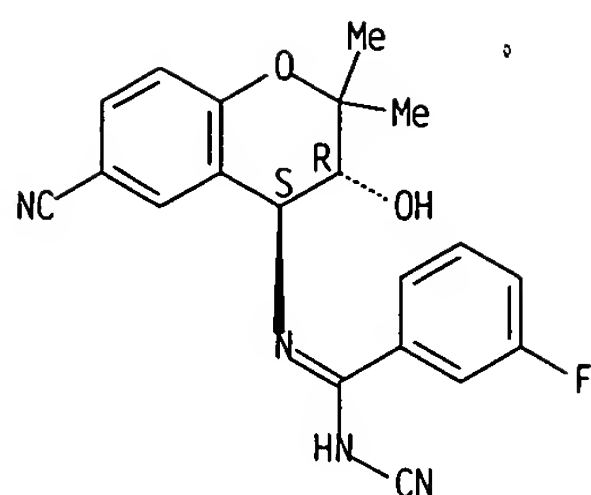
RN 149278-63-7 HCAPLUS
 CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-2-fluoro-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



RN 149278-64-8 HCAPLUS
 CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-3-fluoro-, trans- (9CI) (CA INDEX NAME)

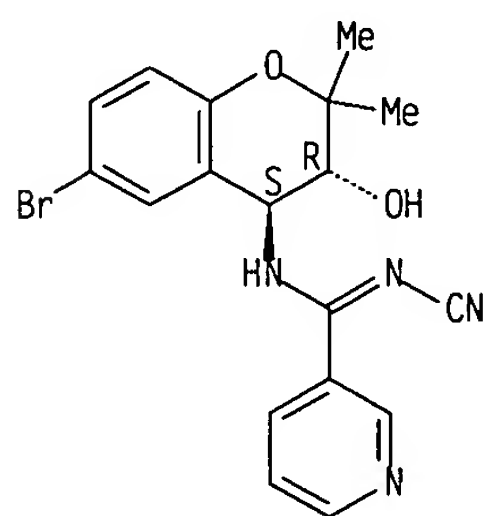
Relative stereochemistry.
 Double bond geometry unknown.



RN 149278-65-9 HCAPLUS

CN 3-Pyridinecarboximidamide, N-(6-bromo-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

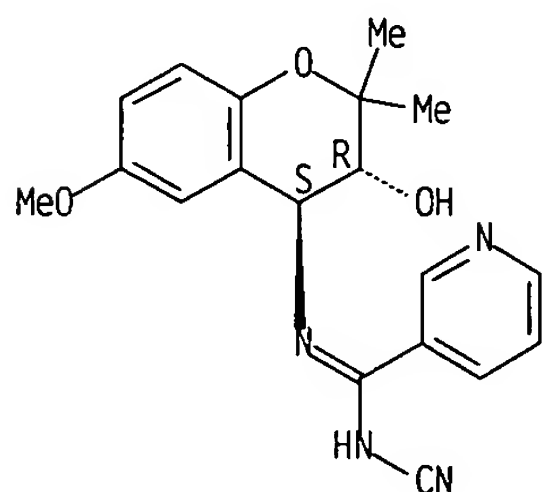
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-66-0 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

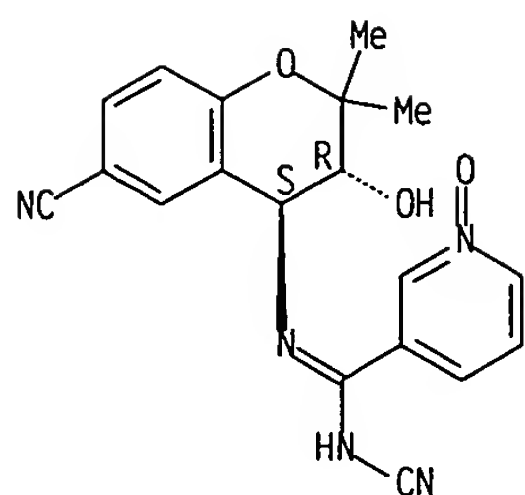
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-67-1 HCAPLUS

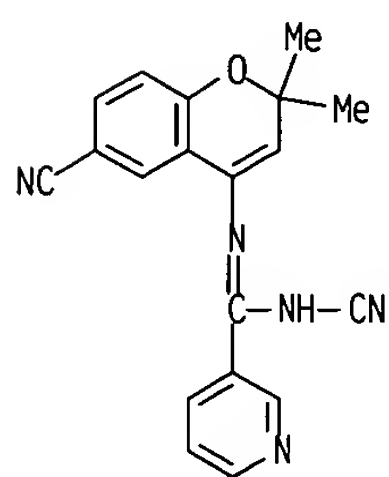
CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, 1-oxide, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RN 149278-68-2 HCAPLUS

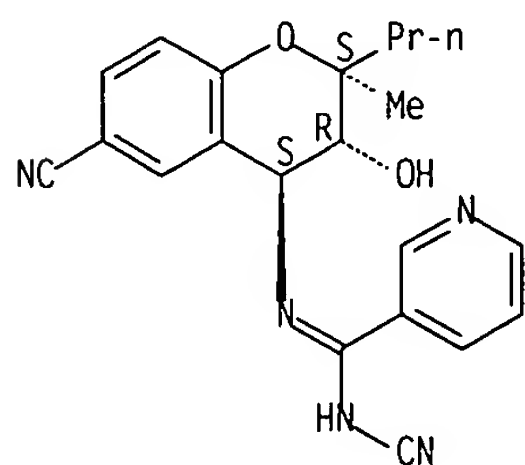
CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 149278-69-3 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2-methyl-2-propyl-2H-1-benzopyran-4-yl)-, (2.alpha.,3.beta.,4.alpha.)- (9CI) (CA INDEX NAME)

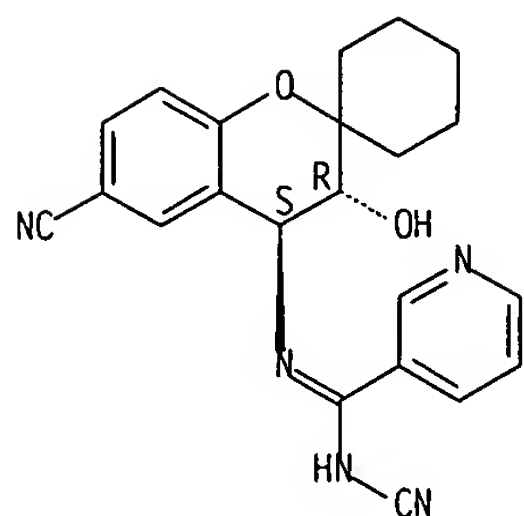
Relative stereochemistry.
Double bond geometry unknown.



RN 149278-70-6 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxyspiro[2H-1-benzopyran-2,1'-cyclohexan]-4-yl)-, trans- (9CI) (CA INDEX NAME)

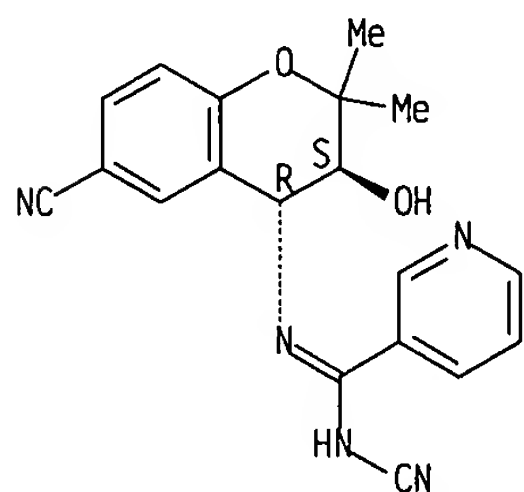
Relative stereochemistry.
Double bond geometry unknown.



RN 149342-19-8 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, (3S-trans)- (9CI) (CA INDEX NAME)

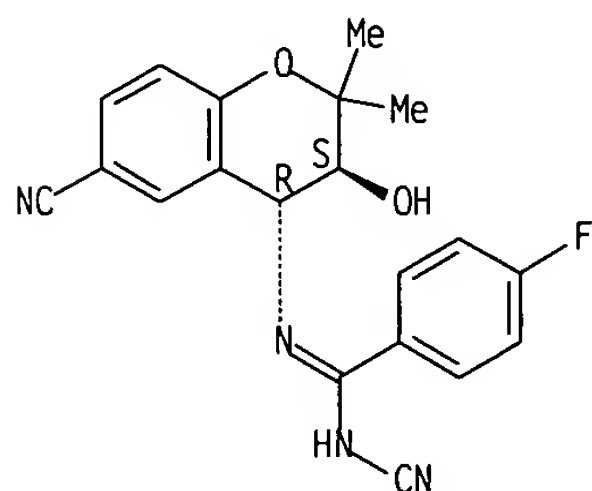
Absolute stereochemistry.
Double bond geometry unknown.



RN 149342-20-1 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-fluoro-, (3S-trans)- (9CI) (CA INDEX NAME)

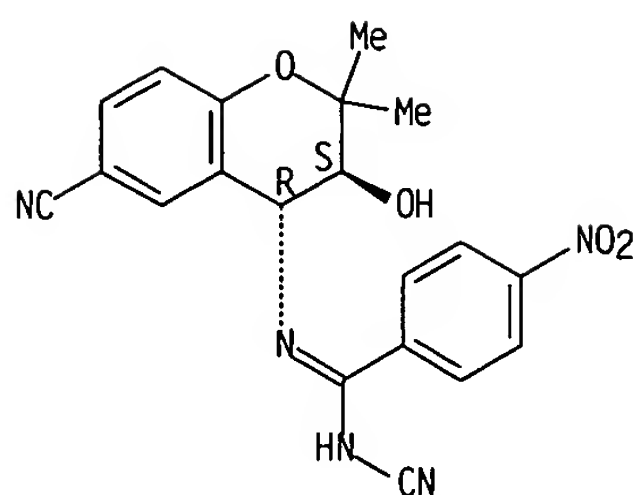
Absolute stereochemistry.
Double bond geometry unknown.



RN 149342-21-2 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-nitro-, (3S-trans)- (9CI) (CA INDEX NAME)

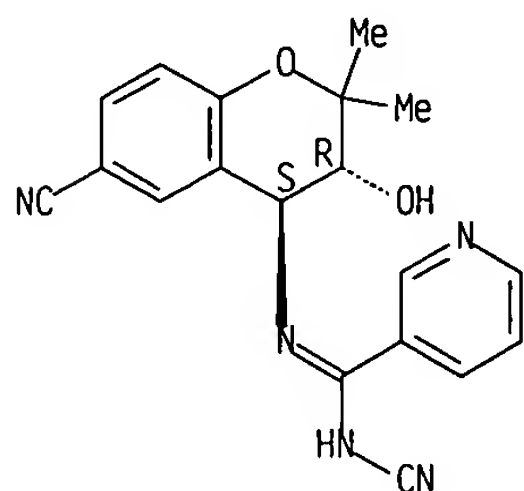
Absolute stereochemistry.
Double bond geometry unknown.



RN 149342-22-3 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, (3R-trans)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



IT 149278-79-5P 149278-88-6P

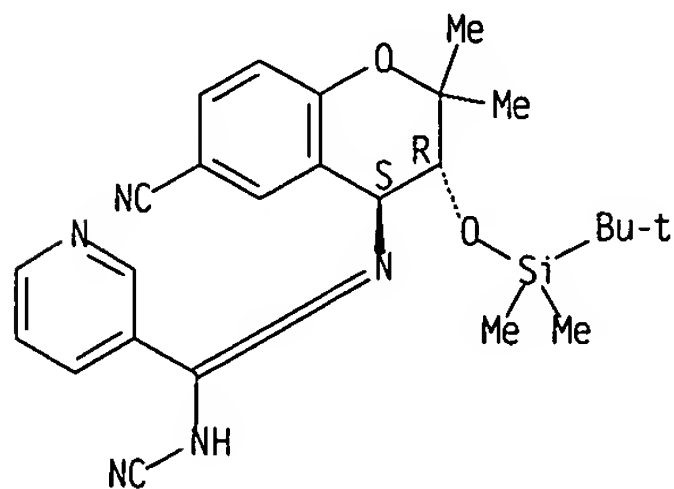
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for antihypertensives and vasodilators)

RN 149278-79-5 HCAPLUS

CN 3-Pyridinecarboximidamide, N-cyano-N'-(6-cyano-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

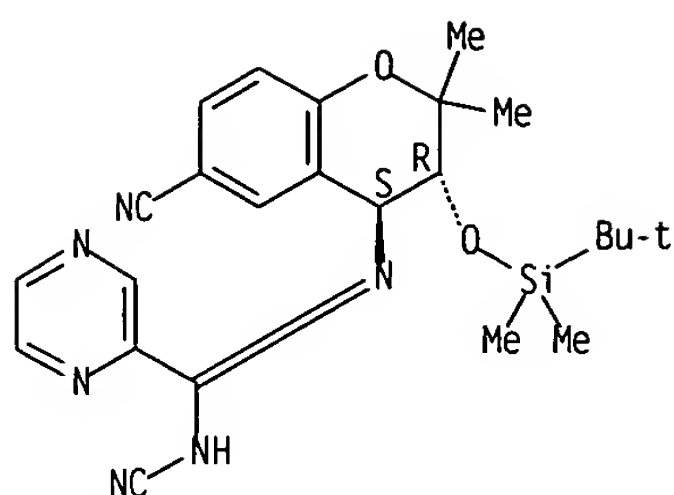
Relative stereochemistry.
Double bond geometry unknown.



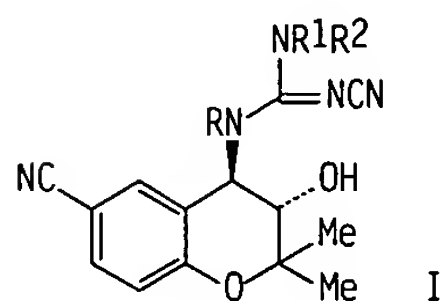
RN 149278-88-6 HCAPLUS

CN Pyrazinecarboximidamide, N-cyano-N'-(6-cyano-3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



L24 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1993:539019 HCAPLUS
 DN 119:139019
 ED Entered STN: 02 Oct 1993
 TI Benzopyranylcyanoguanidine potassium channel openers
 AU Atwal, Karnail S.; Moreland, Suzanne; McCullough, John R.; Ahmed, Syed Z.;
 Normandin, Diane E.
 CS Bristol-Myers Squibb Pharm. Res. Inst., Princeton, NJ, 08543-4000, USA
 SO Bioorganic & Medicinal Chemistry Letters (1992), 2(1), 87-90
 CODEN: BMCLE8; ISSN: 0960-894X
 DT Journal
 LA English
 CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 GI



AB To further investigate whether the K channel openers cromakalim and pinacidil share common pharmacophoric features, the cromakalim analogs I [RR1 = CH2CH2, (CH2)3, R2 = H; R = R2 = H, R1 = H, Me, Et, CHMe2, CMe2Et, CH2CH2NMe2, CH2CH2OMe; R = H, NR1R2 = NMe2, pyrrolidino, N-benzylpiperazino] were prepared. The potent vasodilating activity displayed by I, especially I (R = H, NR1R2 = pyrrolidino), supports the hypothesis of shared pharmacophoric features.
 ST pharmacophore cromakalim pinacidil; benzopyranylcyanoguanidine potassium channel opener; cyanoguanidine benzopyranyl potassium channel opener; antihypertensive benzopyranylcyanoguanidine; vasodilator benzopyranylcyanoguanidine
 IT Antihypertensives
 Vasodilators
 (benzopyranylcyanoguanidines)
 IT Pharmacophores
 (shared pharmacophoric features in cromakalim and pinacidil)
 IT Ion channel openers
 (potassium, benzopyranylcyanoguanidines)
 IT 129462-66-4P 130228-87-4P 134017-89-3P 134017-94-0P 134017-95-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (intermediate in preparation of benzopyranylcyanoguanidine potassium channel openers)
 IT 60560-33-ODP, Pinacidil, benzopyran analogs 94470-67-4DP, Cromakalim, cyanoguanidine analogs 127249-54-1P 127249-61-0P 127249-68-7P

127249-69-8P 127249-70-1P 127249-71-2P 127249-72-3P
 127249-80-3P 134017-78-0P 134017-81-5P 134017-82-6P
 134017-84-8P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and vasodilator activity)

IT 107-15-3P. Ethylenediamine, reactions 109-76-2P. 1,3-Propanediamine
 10191-60-3P. Dimethyl cyanoiminodithiocarbonate 65018-90-8P
 86776-58-1P 127749-52-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (reactant in preparation of benzopyranylcyanoguanidine potassium channel
 openers)

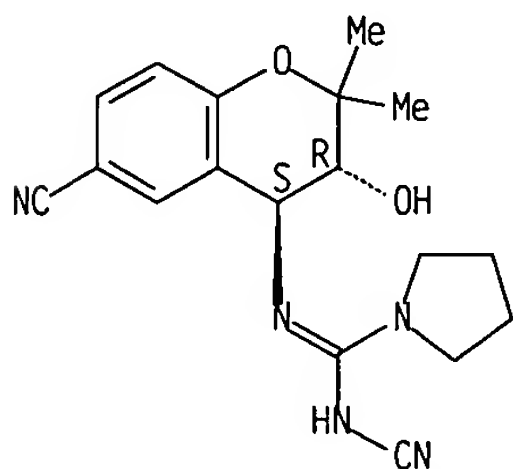
IT 127249-72-3P 134017-82-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and vasodilator activity)

RN 127249-72-3 HCAPLUS

CN 1-Pyrrolidinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-
 2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

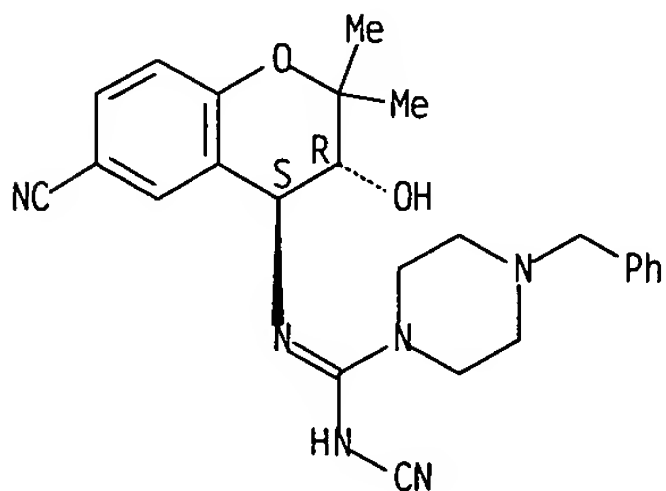
Relative stereochemistry.
 Double bond geometry unknown.



RN 134017-82-6 HCAPLUS

CN 1-Piperazinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-
 dimethyl-2H-1-benzopyran-4-yl)-4-(phenylmethyl)-, trans- (9CI) (CA INDEX
 NAME)

Relative stereochemistry.
 Double bond geometry unknown.



L24 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:495539 HCAPLUS

DN 119:95539

ED Entered STN: 04 Sep 1993

TI Heterocyclyl group-substituted tetralones having antihypertensive and
 bronchodilating activity

IN Almansa, Carmen; Gonzalez, M. Concepcion; Torres, M. Carmen; Carceller,
 Elena; Bartroli, Javier

PA Uriach, J., e Cia. S.A., Spain

SO Eur. Pat. Appl., 39 pp.

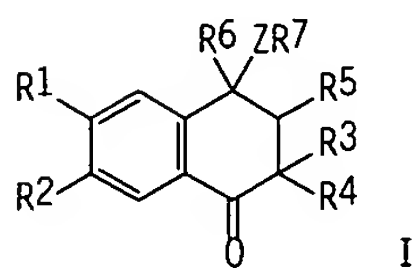
CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07D237-16
 ICS C07D239-42; C07C255-56; C07C255-60; C07D213-64; C07D213-81;
 C07D307-68; A61K031-395
 CC 28-15 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 1
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | EP 525768 | A1 | 19930203 | EP 1992-113007 | 19920730 <-- |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE | | | | |
| | ES 2033581 | A1 | 19930316 | ES 1991-1777 | 19910730 <-- |
| | ES 2033581 | B1 | 19931216 | | |
| | ES 2041212 | A1 | 19931101 | ES 1992-333 | 19920217 <-- |
| | ES 2041212 | B1 | 19940516 | | |
| | CA 2074864 | AA | 19930131 | CA 1992-2074864 | 19920729 <-- |
| PRAI | ES 1991-1777 | A | 19910730 | <-- | |
| | ES 1992-333 | A | 19920217 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|--|
| EP 525768 | ICM | C07D237-16 |
| | ICS | C07D239-42; C07C255-56; C07C255-60; C07D213-64; C07D213-81; C07D307-68; A61K031-395 |

OS MARPAT 119:95539
 GI



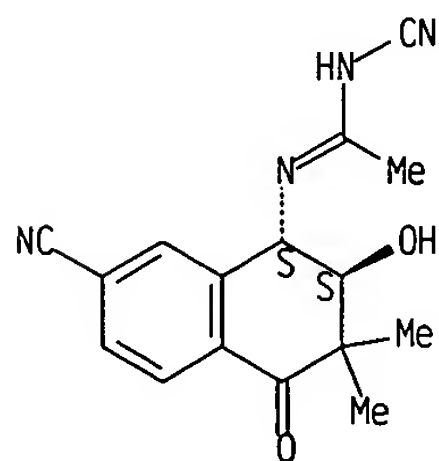
AB The title compds. I [R1, R2 = H, OH, CHO, CO2H, NO2, NH2CN, halogen, OCF3, alkoxy, C.tplbond.CH, (un)substituted alkylcarbonyl, arylsulfinyl, alkylsulfinyl, arylsulfonyl, alkyl, alkylsulfonylamino, aminosulfinyl, aminosulfonyl, etc.; R3 = H, alkyl; R4 = alkyl; R5 = OH, acetoxy, formyloxy; R6 = H, olefinic bond with R5; Z = O, NR8; R3R4 = C2-5 methylene chain; if Z = O, then R7 = R9 where R9 = C3-6 cycloalkyl, C3-6 cycloalkenyl, Ph, heteroaryl (all optionally substituted by 1-2 halogen atoms and/or 1-2 C1-6 alkyl, C1-6 alkoxy, arylmethoxy, etc., but when Z = NR8, then R7 = R9, C(:X)R10; R10 = H, (un)substituted C1-6 alkyl, C2-6 alkenyl, C3-6 cycloalkyl, (un)substituted Ph, (un)substituted heteroaryl; X = O, S, NCN], useful as antihypertensive and bronchodilating agents, are prepared Thus, 3,4-epoxy-2,2-dimethyl-1-oxo-1,2,3,4-tetrahydronaphthalene-6-carbonitrile reacted with 3,6-dihydropyridazine to give trans-2,2-dimethyl-3-hydroxy-4-(6-hydroxy-3-pyridazinyloxy)-1-oxo-1,2,3,4-tetrahydronaphthalene-6-carbonitrile (II) in 65% yield. In spontaneously hypertensive rats at 1 mg/kg, II lowered arterial blood pressure 116 mm Hg, and at 8.8 .mu.M inhibited 50% noradrenaline-induced contraction in portal vein isolated from rat.

ST antihypertensive tetralone prepn; bronchodilation tetralone prepn; hypertension treatment tetralone drug; asthma treatment tetralone drug; pyridazinyloxytetralone antihypertensive agent; pyridazinyloxytetrahydronaphthalenecarbonitrile bronchodilating agent

IT Antihypertensives
 Bronchodilators
 (heterocycl-yl-substituted tetralones)

- IT 148925-41-1P 148925-42-2P 148925-43-3P 148925-45-5P 148925-46-6P
 148925-47-7P 148925-48-8P 148925-49-9P 148925-51-3P 148925-52-4P
 148925-53-5P 148925-54-6P 148925-55-7P 148925-57-9P 148925-58-0P
 148925-59-1P 148925-60-4P 148925-61-5P 148925-62-6P 148925-63-7P
 148925-64-8P 148925-65-9P 148925-66-0P 148925-67-1P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and antihypertensive and bronchodilating activity of)
- IT 148925-44-4P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and antihypertensive and bronchodilating activity of, reaction of)
- IT 17257-71-5P 32281-97-3P, 7-Bromo-1,2,3,4-Tetrahydronaphthalen-1-one
 148925-37-5P, 7-Bromo-2,2-dimethyl-1,2,3,4-tetrahydronaphthalen-1-one
 148925-38-6P, 7-Bromo-2,2-dimethyl-1,2-dihydronaphthalen-1-one
 148925-39-7P, 7-Bromo-2,2-dimethyl-3,4-epoxy-1,2,3,4-tetrahydronaphthalen-1-one
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, in preparation of antihypertensive and bronchodilating tetralones)
- IT 55-22-1, 4-Pyridinecarboxylic acid, reactions 59-67-6, Nicotinic acid, reactions 65-85-0, Benzoic acid, reactions 98-98-6, 2-Pyridinecarboxylic acid 100-09-4, 4-Methoxybenzoic acid 106-95-6, Allyl bromide, reactions 123-33-1, 3,6-Dihydropyridazine 488-93-7, 3-Furoic acid 1193-21-1, 4,6-Dichloropyrimidine 3859-41-4, 1,3-Cyclopentanedione 5231-87-8, 3,4-Diethoxycyclobutene-1,2-dione 56563-07-6 72762-00-6, 2-Hydroxypyridine 148925-40-0 148925-50-2, 6-Bromo-2,2-dimethyl-3,4-epoxy-1,2,3,4-tetrahydronaphthalen-1-one 149455-94-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of antihypertensive and bronchodilating tetralones)
- IT 148925-65-9P
 RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation and antihypertensive and bronchodilating activity of)
- RN 148925-65-9 HCAPLUS
- CN Ethanimidamide, N-cyano-N'-(7-cyano-1,2,3,4-tetrahydro-2-hydroxy-3,3-dimethyl-4-oxo-1-naphthalenyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



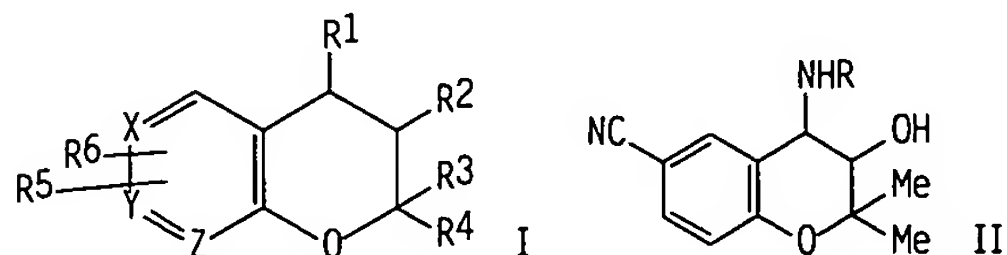
L24 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1993:212894 HCAPLUS
 DN 118:212894
 ED Entered STN: 29 May 1993
 TI Preparation of benzopyranylcyanoguanidine derivatives
 IN Atwal, Karnail; Grover, Gary J.; Kim, Kyoung S.

PA E. R. Squibb and Sons, Inc., USA
 SO U.S., 25 pp. Cont.-in-part of U.S. Ser. No. 506.632. abandoned.
 CODEN: USXXAM
 DT Patent
 LA English
 IC ICM C07D471-02
 ICS C07D409-14; C07D311-96; C07D417-04; C07D405-14; A61K031-35;
 A61K031-66
 NCL 514302000
 CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1
 FAN.CNT 5

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | US 5140031 | A | 19920818 | US 1991-661763 | 19910227 <-- |
| | ZA 9003491 | A | 19910227 | ZA 1990-3491 | 19900508 <-- |
| | IN 173988 | A | 19940820 | IN 1990-DE494 | 19900522 <-- |
| | DD 294715 | A5 | 19911010 | DD 1990-341153 | 19900530 <-- |
| | PL 165385 | B1 | 19941230 | PL 1990-290038 | 19900531 <-- |
| | IN 178152 | A | 19970308 | IN 1992-DE96 | 19920207 <-- |
| | CA 2061699 | AA | 19920828 | CA 1992-2061699 | 19920224 <-- |
| | CA 2061699 | C | 20020521 | | |
| | AU 9211147 | A1 | 19920903 | AU 1992-11147 | 19920224 <-- |
| | AU 650512 | B2 | 19940623 | | |
| | ZA 9201333 | A | 19921125 | ZA 1992-1333 | 19920224 <-- |
| | NO 9200767 | A | 19920828 | NO 1992-767 | 19920226 <-- |
| | NO 180679 | B | 19970217 | | |
| | NO 180679 | C | 19970528 | | |
| | EP 501797 | A1 | 19920902 | EP 1992-301654 | 19920227 <-- |
| | EP 501797 | B1 | 19960605 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, MC, NL, PT, SE | | | | |
| | CN 1064272 | A | 19920909 | CN 1992-101340 | 19920227 <-- |
| | CN 1035253 | B | 19970625 | | |
| | AT 138919 | E | 19960615 | AT 1992-301654 | 19920227 <-- |
| | ES 2088537 | T3 | 19960816 | ES 1992-301654 | 19920227 <-- |
| | IN 180495 | A | 19980207 | IN 1992-DE1111 | 19921126 <-- |
| PRAI | US 1989-359236 | B2 | 19890531 | <-- | |
| | US 1990-493060 | B2 | 19900313 | <-- | |
| | US 1990-506632 | B2 | 19900409 | <-- | |
| | IN 1990-DE494 | A1 | 19900522 | <-- | |
| | US 1991-661763 | A | 19910227 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|--------|---|
| US 5140031 | ICM | C07D471-02 |
| | ICS | C07D409-14; C07D311-96; C07D417-04; C07D405-14; A61K031-35; A61K031-66 |
| | NCL | 514302000 |
| EP 501797 | ECLA | C07D311/68; C07D311/70; C07F009/655P60 <-- |
| OS | MARPAT | 118:212894 |
| GI | | |



AB Title compds. I [X,Y,Z = CH or 1 of them = N, NO and the others = CH; R1 = R7R8NC(:NCN)NR9 wherein R7 = aryl, heterocyclyl, heterocyclylalkyl, R8 = H, alkyl, aryl, alkenyl, arylalkyl, R9 = H, alkyl, alkenyl, alkenyl, aryl,

arylalkyl, cycloalkyl, cycloalkylalkyl; R2 = H, HO, OAc; R3, R4 = H, alkyl, arylalkyl; R3R4 = 5-7-membered carbocyclyl; R5 = H, alkyl, haloalkyl, alkenyl, alkynyl, etc.; R6 = H, alkyl, HO, alkoxy, (substituted) amino, etc.] having K-channel activity useful as antiischemic agents (no data), are prepared Aminobenzopyran trans-II (R = H) was condensed with NCNHCSNHMe2Et (preparation given) to give trans-II [R = NHC(:NCN)NHMe2Et].

ST cyanoguanidine cyanohydroxybenzopyranyl prepn cardiovascular;
benzopyranylcyanoguanidine prepn antiischemic; potassium channel activator
benzopyranylcyanoguanidine

IT Cardiovascular agents
(benzopyranylcyanoguanidines)

IT Ischemia
(treatment of, benzopyranylcyanoguanidines for)

IT Ion channel openers
(potassium, benzopyranylcyanoguanidines)

IT 41835-08-9P 89125-07-5P 98557-54-1P 118581-55-8P 127419-05-0P
127749-51-3P 127749-52-4P 127779-17-3P 127806-70-6P 129180-58-1P
129180-59-2P 129462-66-4P 129462-74-4P 129462-75-5P 130228-87-4P
132685-98-4P 134017-90-6P 134017-91-7P 134017-92-8P 134017-93-9P
134017-94-0P 134017-96-2P 134017-97-3P 134017-99-5P 134018-01-2P
134028-71-0P 134828-12-9P 144264-59-5P 144264-60-8P 144264-61-9P
144264-62-0P 144264-63-1P 144264-64-2P 144264-65-3P 146941-85-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent)

(preparation and reaction of, in preparation of cardiovascular agents)

IT 127249-61-0P 127249-68-7P 127249-69-8P 127249-70-1P 127249-71-2P
127249-72-3P 130228-92-1P 130228-95-4P 133178-30-0P
134017-78-0P 134017-79-1P 134017-80-4P 134017-81-5P
134017-82-6P 134017-83-7P 134017-84-8P 134017-85-9P
134017-86-0P 134017-87-1P 134017-88-2P 134035-97-5P 134053-73-9P
134053-74-0P 144264-44-8P 144264-45-9P 144264-46-0P 144264-51-7P
144264-52-8P 144264-53-9P 144264-54-0P 144301-93-9P 144301-94-0P
144301-95-1P 146941-74-4P 146941-75-5P 146941-76-6P 146941-77-7P
146941-78-8P 146941-79-9P 146941-80-2P 146941-81-3P 146941-82-4P
146941-83-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as cardiovascular agent)

IT 75-31-0, 2-Propanamine, reactions 100-46-9, Benzylamine, reactions
103-72-0, Phenyl isothiocyanate 107-15-3, 1,2-Ethanediamine, reactions
109-76-2, 1,3-Diaminopropane 109-85-3 123-75-1, Pyrrolidine, reactions
506-59-2, Dimethylaminehydrochloride 536-74-3, Phenylacetylene
540-38-5, 4-Iodophenol 542-85-8, Ethyl isothiocyanate 557-66-4,
Ethylaminehydrochloride 611-71-2, (R)(-)-Mandelic acid 628-03-5
811-93-8, 1,1-Dimethylethylenediamine 1111-97-3, 3-Chloro-3-methyl-1-
butyne 1544-68-9, 4-Fluorophenyl isothiocyanate 1645-65-4,
4-Trifluoromethylphenyl isothiocyanate 2131-55-7, 4-Chlorophenyl
isothiocyanate 2131-61-5, (4-Nitrophenyl)isothiocyanate 2284-20-0,
4-Methoxyphenyl isothiocyanate 2392-68-9, 3-Chlorophenylisothiocyanate
2740-81-0, 2-Chlorophenyl isothiocyanate 2759-28-6 3731-51-9,
2-(Aminomethyl)pyridine 3731-52-0, 3-(Aminomethyl)pyridine 3731-53-1,
4-(Aminomethyl)pyridine 4788-37-8 6590-94-9, 3,4-Dichlorophenyl
isothiocyanate 10191-60-3 16035-50-0 17199-29-0 17292-62-5,
Monosodium cyanamide 33143-29-2 65018-90-8 79463-77-7, Diphenyl
cyanocarbonimidate 86776-58-1 86823-96-3 108031-11-4 139674-35-4
139768-71-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of cardiovascular agents)

IT 127249-72-3P 134017-82-6P

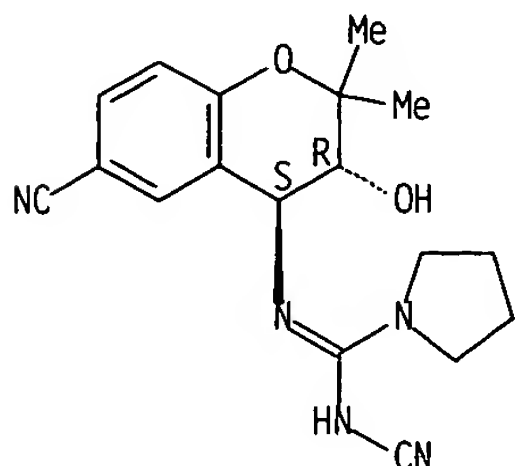
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as cardiovascular agent)

RN 127249-72-3 HCAPLUS

CN 1-Pyrrolidinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

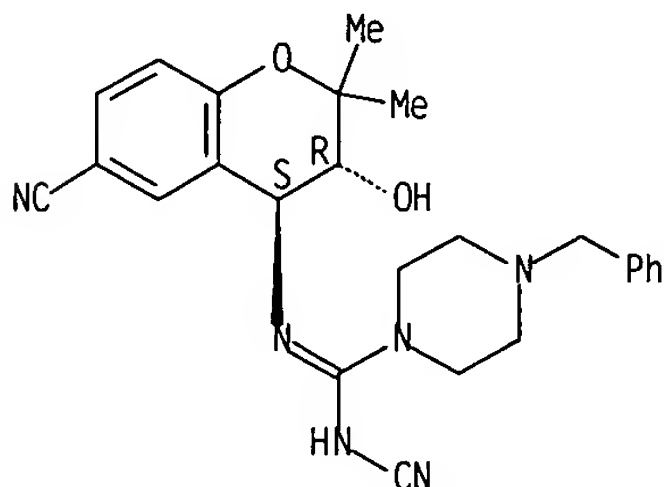
Relative stereochemistry.
Double bond geometry unknown.



RN 134017-82-6 HCAPLUS

CN 1-Piperazinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-(phenylmethyl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



L24 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1993:22146 HCAPLUS

DN 118:22146

ED Entered STN: 24 Jan 1993

TI Preparation of N-cyano-N'-(azabicycloalkyl)indolineiminocarboxamides and analogs as 5HT3 receptor antagonists

IN King, Francis David; Gaster, Laramie Mary

PA SmithKline Beecham PLC. UK

SO PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DT Patent

LA English

IC ICM C07D451-04

ICS C07D491-08; A61K031-46

ICI C07D491-08, C07D265-00, C07D221-00

CC 27-16 (Heterocyclic Compounds (One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|--|------|----------|-----------------|--------------|
| PI | WO 9214733 | A1 | 19920903 | WO 1992-GB310 | 19920220 <-- |
| | W: AU, CA, JP, KR, RU, US | | | | |
| | RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, MC, NL, SE | | | | |

AU 9212095 A1 19920915 AU 1992-12095 19920220 <--
 PRAI GB 1991-3839 A 19910223 <--
 WO 1992-GB310 A 19920220 <--

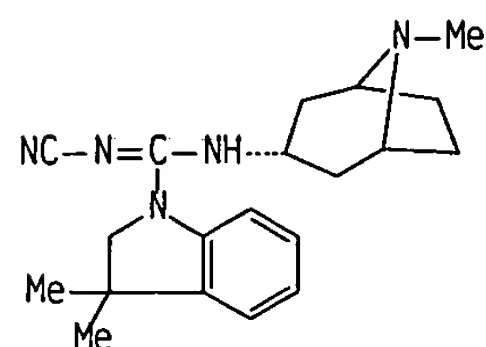
CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

WO 9214733 ICM C07D451-04
 ICS C07D491-08; A61K031-46
 ICI C07D491-08, C07D265-00, C07D221-00

OS MARPAT 118:22146

GI



I

AB XC(:Y)NHZ [X = (anellated) Ph, -heteroaryl; Y = NCN, NR1, CR1; R1 = NO2, COR2, SO2R2; R2 = alkyl, NH2, alkylamino, (substituted) Ph; Z = diazacycloalkyl, azabicycloalkyl] were prepared as 5HT3 receptor antagonists (no data). Thus, 3,3-dimethylindoline was condensed with (MeS)2C:NCN and the product condensed with 8-methyl-8-azabicyclo[3.2.1]octan-3-amine to give endo-I.

ST indolinylinocarboxamide prepn 5HT receptor antagonist

IT Analgesics
 Antiemetics
 Nervous system agents
 (N-cyano-N'-(azabicycloalkyl)indolineiminocarboxamides and analogs)

IT Digestive tract
 (disease, treatment of, N-cyano-N'-(azabicycloalkyl)indolineiminocarboxamides and analogs for)

IT 145127-19-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, in preparation of 5-HT receptor antagonist)

IT 145127-16-8P 145127-17-9P 145127-18-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as 5-HT receptor antagonist)

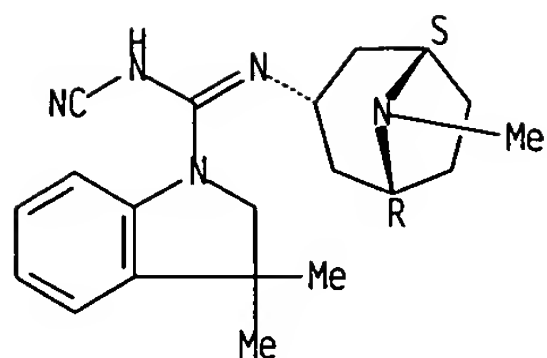
IT 1914-02-9, 3,3-Dimethylindoline 10191-60-3 66031-28-5,
 1,1-Bis(methylthio)-2-nitroethane 87571-88-8 130914-52-2
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of 5-HT receptor antagonist)

IT 145127-16-8P 145127-18-0P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as 5-HT receptor antagonist)

RN 145127-16-8 HCAPLUS

CN 1H-Indole-1-carboximidamide, N-cyano-2,3-dihydro-3,3-dimethyl-N'-(8-methyl-8-azabicyclo[3.2.1]oct-3-yl)-, endo- (9CI) (CA INDEX NAME)

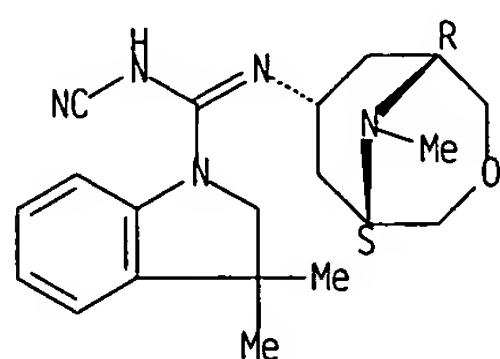
Relative stereochemistry.
 Double bond geometry unknown.



RN 145127-18-0 HCAPLUS

CN 1H-Indole-1-carboximidamide, N-cyano-2,3-dihydro-3,3-dimethyl-N'-(9-methyl-3-oxa-9-azabicyclo[3.3.1]non-7-yl)-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



L24 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1992:255603 HCAPLUS

DN 116:255603

ED Entered STN: 27 Jun 1992

TI Preparation of pyridylpyrrolothiazole derivatives as platelet activating factor (PAF) antagonists

IN Mase, Toshiyasu; Kondo, Yutaka; Nagaoka, Hitoshi; Yamada, Toshimitsu; Tomioka, Kenichi

PA Yamanouchi Pharmaceutical Co., Ltd., Japan

SO Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DT Patent

LA Japanese

IC ICM C07D513-04

ICS A61K031-425

CC 28-7 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 1

FAN.CNT 1

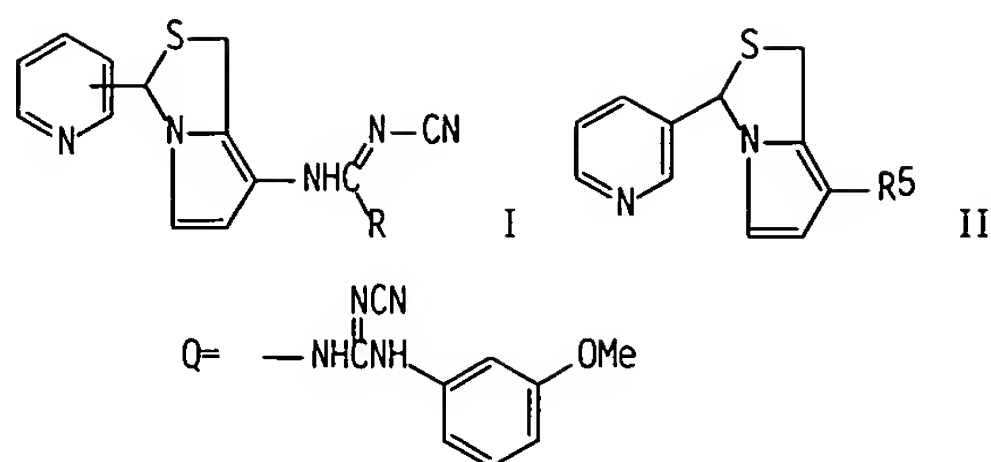
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---------------|------|----------|-----------------|--------------|
| PI | JP 03287587 | A2 | 19911218 | JP 1990-90960 | 19900404 <-- |
| PRAI | JP 1990-90960 | | 19900404 | <-- | |

CLASS

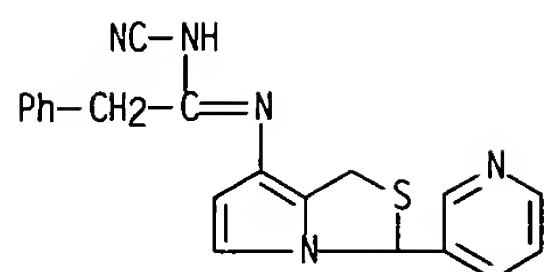
| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|-------------|-------|------------------------------------|
| JP 03287587 | ICM | C07D513-04 |
| | ICS | A61K031-425 |

OS MARPAT 116:255603

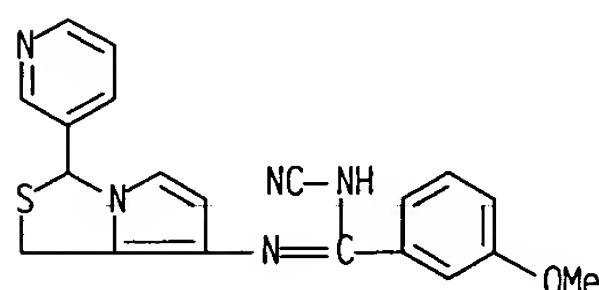
GI



- AB The title compds. (I; R = NR₁R₂; R₁, R₂ = H, alkyl, XC₆H₄R₃; X = single bond, alkylene; R₃ = H, alkyl, OH, alkoxy, aralkyloxy, aryloxy, acyl) and their intermediate isourea derivs. I [R = YR₄; Y = O, S; R₄ = lower alkyl or (un)substituted Ph], which themselves also show anti-PAF activity, are prepared. Thus, acylation of a pyrrolo[1,2-c]thiazole derivative (II; R₅ = NH₂) with di-Ph N-cyanocarbonimidate in 2-propanol at 90.degree. overnight and condensation of the resulting II [R₅ = NHC(:NCN)OPh] with 4-phenylbutylamine in 2-propanol at 90.degree. overnight gave II [R₅ = NHC(:NCN)NH(CH₂)₄Ph]. II (R₅ = Q) in vitro inhibited PAF-induced coagulation of rabbit blood platelets with IC₅₀ of 4.5 .times. 10⁻⁸ M. Addnl. 8 I were prepared
- ST pyridylpyrrolothiazolylguanidine prepn PAF antagonist; pyrrolothiazole pyridyl guanidino PAF antagonist; platelet activating factor antagonist
- IT 79463-77-7, Diphenyl N-cyanocarbonimidate
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminopyrrolothiazole derivative)
- IT 135611-15-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of, by di-ph N-cyanocarbonimidate)
- IT 65154-06-5, Platelet activating factor
RL: RCT (Reactant); RACT (Reactant or reagent)
(antagonists, (pyridylpyrrolothiazolyl)guanidine derivs.)
- IT 64-04-0, Phenethylamine 100-46-9, Benzylamine, reactions 104-94-9, p-Anisidine 107-10-8, 1-Propylamine, reactions 536-90-3, m-Anisidine 2835-78-1 3586-12-7, m-Phenoxyaniline 13214-66-9, 4-Phenylbutylamine 41406-00-2, m-Isopropoxyaniline
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with O-phenyl-N'-pyrrolothiazolylisourea derivative)
- IT 141187-35-1P 141187-36-2P 141187-37-3P **141187-38-4P**
141187-39-5P **141187-40-8P** 141187-41-9P 141187-42-0P
141187-43-1P 141187-44-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as platelet activating factor antagonist)
- IT **141187-38-4P 141187-40-8P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as platelet activating factor antagonist)
- RN 141187-38-4 HCAPLUS
- CN Benzeneethanimidamide, N-cyano-N'-[3-(3-pyridinyl)-1H,3H-pyrrolo[1,2-c]thiazol-7-yl]- (9CI) (CA INDEX NAME)



RN 141187-40-8 HCAPLUS
 CN Benzenecarboximidamide, N-cyano-3-methoxy-N'-[3-(3-pyridinyl)-1H-pyrrolo[1,2-c]thiazol-7-yl]- (9CI) (CA INDEX NAME)



L24 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1991:449406 HCAPLUS
 DN 115:49406
 ED Entered STN: 10 Aug 1991
 TI Preparation of 6-cyano-2,2-dimethyl-4-[(N-cyanoimidoyl)amino]-2H-benzo[b]pyrans and analogs as antihypertensives and bronchodilators
 IN Ohtuka, Katuyuki; Ishiyama, Nobuo; Iida, Yasuhito; Seri, Kenji; Murai, Takeshi; Sanai, Kazuko; Ishizaka, Yoshihiro
 PA Kaken Pharmaceutical Co., Ltd., Japan
 SO Eur. Pat. Appl., 41 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07D311-68
 ICS A61K031-35
 CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1, 63

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | EP 412531 | A1 | 19910213 | EP 1990-115242 | 19900808 <-- |
| | EP 412531 | B1 | 19940511 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | US 5095016 | A | 19920310 | US 1990-562577 | 19900803 <-- |
| | CA 2022882 | AA | 19910212 | CA 1990-2022882 | 19900808 <-- |
| | AT 105556 | E | 19940515 | AT 1990-115242 | 19900808 <-- |
| | AU 9060844 | A1 | 19910214 | AU 1990-60844 | 19900809 <-- |
| | AU 624526 | B2 | 19920611 | | |
| | NO 9003524 | A | 19910212 | NO 1990-3524 | 19900810 <-- |
| | NO 174050 | B | 19931129 | | |
| | NO 174050 | C | 19940309 | | |
| | HU 54673 | A2 | 19910328 | HU 1990-4956 | 19900810 <-- |
| | JP 03279377 | A2 | 19911210 | JP 1990-213529 | 19900810 <-- |
| | JP 3037979 | B2 | 20000508 | | |
| | JP 03279378 | A2 | 19911210 | JP 1990-213530 | 19900810 <-- |
| | JP 3037980 | B2 | 20000508 | | |
| | CN 1049500 | A | 19910227 | CN 1990-107121 | 19900811 <-- |
| PRAI | JP 1989-208547 | A | 19890811 | <-- | |
| | JP 1989-341528 | A | 19891229 | <-- | |
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| | JP 1990-73654 | A | 19900323 | <-- | |

EP 1990-115242 A 19900808 <--

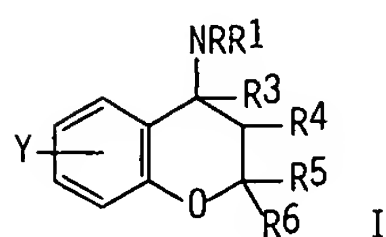
CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

EP 412531 ICM C07D311-68
ICS A61K031-35

OS MARPAT 115:49406

GI



- AB Title compds. [I: R = R₂C:NCN; R₁ = H, (un) substituted alkyl, alkenyl, alkynyl, R₇CO; R₂ = (substituted) alkyl, Ph; R₃ = H; R₄ = OH; R₃R₄ = bond; R₅, R₆ = alkyl; R₇ = alkyl, Ph, alkoxy, (Ph substituted) alkenyl; Y = cyano, halo, NO₂, alkyl(carbonyl), alkynyl, carboxyl, aryl, morpholinocarbonyl, etc.] (II) or their pharmaceutically acceptable salts, were prepared, e.g., by reaction of aminobenzopyranols (I: R = R₁ = H, R₃ = OH, Y .noteq. CO₂H) with R₂(OR₈)C:NCN (R₈ = alkyl, R₂ as above). Thus, a mixture of 1.23 g N-cyanoacetimide and 2.18 g 6-cyano-3,4-dihydro-2,2-dimethyl-trans-4-amino-2H-benzo[b]pyran-3-ol was stirred for 2 h at 100-120.degree. to give 1.75 g title compound (I: R = CMe:NCN, R₁ = R₃ = H, R₄ = OH, R₅ = R₆ = Me, Y = 6-cyano) (III). The latter at 3 mg/kg orally in rats reduced blood pressure to 56% of preadministration values after 3 h. In vitro 3 .times. 10-6M III gave 41.6% relaxation of guinea pig trachial smooth muscle.
- ST cyanodimethylcyanoimidoylaminobenzopyran prepn antihypertensive bronchodilator; benzopyranylaminoimide prepn antihypertensive bronchodilator
- IT Antihypertensives
Bronchodilators
(cyanodimethyl(cyanoimidoylamino)benzopyran and analogs)
- IT 75-36-5, Acetyl chloride
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of aminobenzopyran derivative, in preparation of hypertensive and bronchodilator)
- IT 110-91-8, Morpholine, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of carboxybenzopyran derivative, in preparation of antihypertensive and bronchodilator)
- IT 105-36-2, Ethyl bromoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminobenzopyran derivative, in preparation of antihypertensive and bronchodilator)
- IT 134017-97-3P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and desilylation of, in preparation of antihypertensive and bronchodilator)
- IT **134828-13-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and elimination reaction of, in preparation of antihypertensive and bronchodilator)
- IT 133178-23-1P 133178-25-3P 133178-26-4P
133178-28-6P 133178-29-7P 133178-31-1P
133178-32-2P 133178-35-5P 133178-36-6P
133178-37-7P 133178-41-3P 133178-44-6P

133178-48-0P 133178-50-4P 133178-55-9P
 134827-45-5P 134827-46-6P 134827-47-7P 134827-48-8P
 134827-49-9P 134827-50-2P 134827-51-3P 134827-52-4P
 134827-53-5P 134827-54-6P 134827-55-7P
 134827-56-8P 134827-57-9P 134827-58-0P
 134827-59-1P 134827-60-4P 134827-61-5P
 134827-62-6P 134827-63-7P 134827-64-8P
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 134828-10-7P 134828-11-8P 134828-12-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as antihypertensive and bronchodilator)

IT 1558-82-3 4428-98-2, Ethyl N-cyanoformimidate 33490-49-2 54356-31-9,
 Ethyl N-cyanopropionimidate 54356-33-1 100220-54-0, Ethyl
 N-cyanobutyrimidate

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with aminobenzopyran derivative, in preparation of
 antihypertensive and bronchodilator)

IT 86776-58-1 89316-91-6 134828-14-1 134828-15-2 134828-16-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with cyanoimides, in preparation of antihypertensives and
 bronchodilators)

IT 1066-54-2, Trimethylsilyl acetylene

RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reaction of, with bromobenzopyran derivative, in preparation of
 antihypertensive and bronchodilator)

IT 122262-14-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(substitution reaction of, with silylacetylene, in preparation of
 antihypertensive and bronchodilator)

IT 134828-13-0P

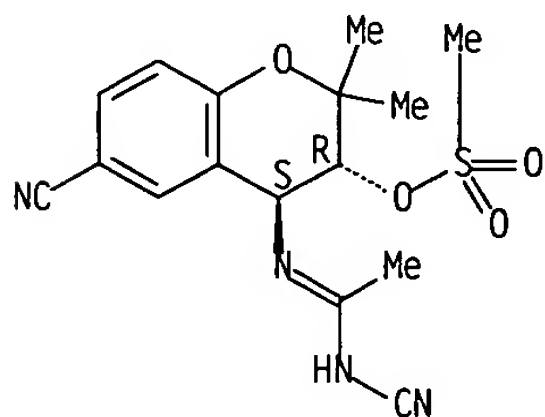
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and elimination reaction of, in preparation of antihypertensive and
 bronchodilator)

RN 134828-13-0 HCAPLUS

CN Ethanimidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2,2-dimethyl-3-
 [(methylsulfonyl)oxy]-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX
 NAME)

Relative stereochemistry.
 Double bond geometry unknown.



IT 133178-23-1P 133178-25-3P 133178-26-4P

133178-28-6P 133178-29-7P 133178-31-1P
 133178-32-2P 133178-35-5P 133178-36-6P
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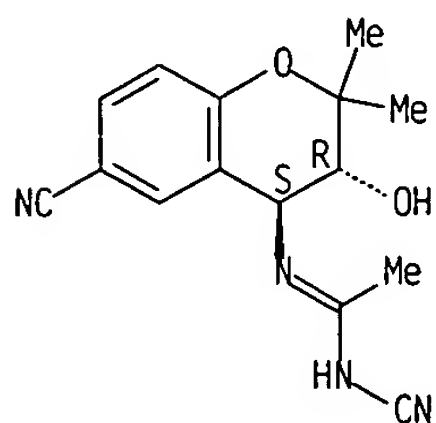
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as antihypertensive and bronchodilator)

RN 133178-23-1 HCAPLUS

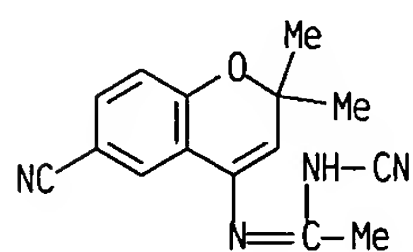
CN Ethanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



RN 133178-25-3 HCAPLUS

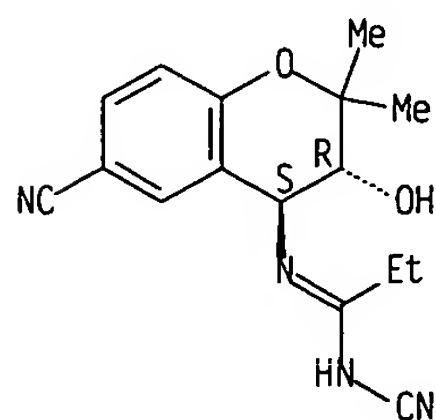
CN Ethanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 133178-26-4 HCAPLUS

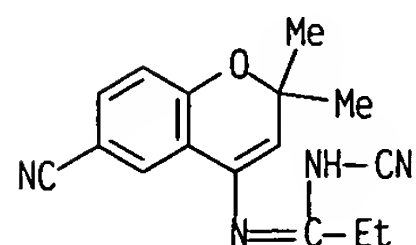
CN Propanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
 Double bond geometry unknown.



RN 133178-28-6 HCAPLUS

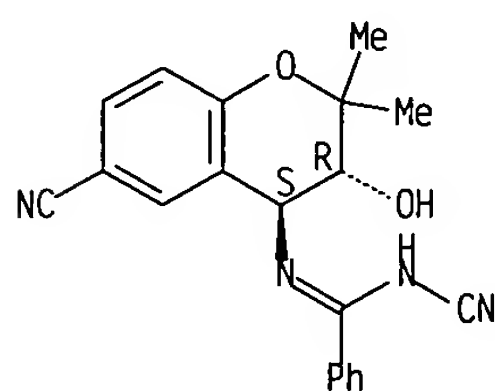
CN Propanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)-
(9CI) (CA INDEX NAME)



RN 133178-29-7 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

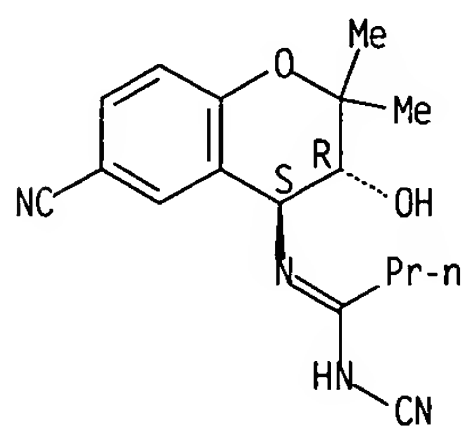
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-31-1 HCAPLUS

CN Butanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

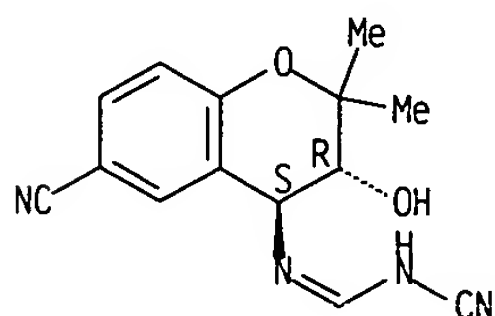
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-32-2 HCAPLUS

CN Methanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

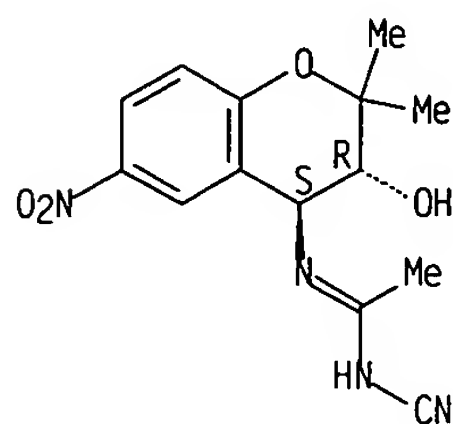
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-35-5 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

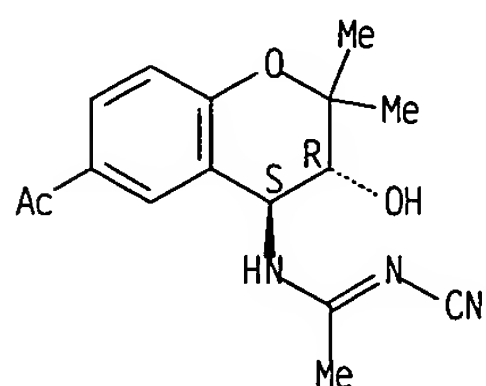
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-36-6 HCAPLUS

CN Ethanimidamide, N-(6-acetyl-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

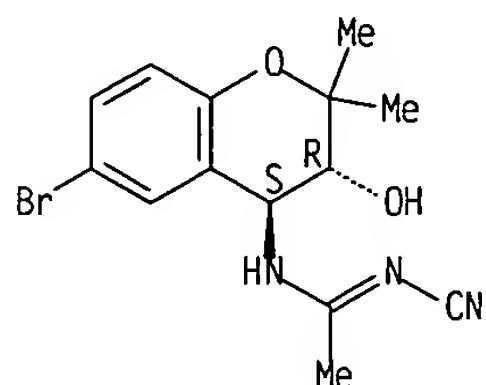
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-37-7 HCAPLUS

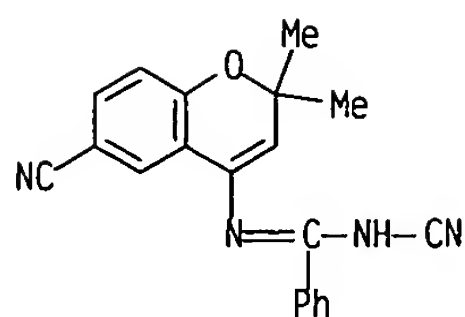
CN Ethanimidamide, N-(6-bromo-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



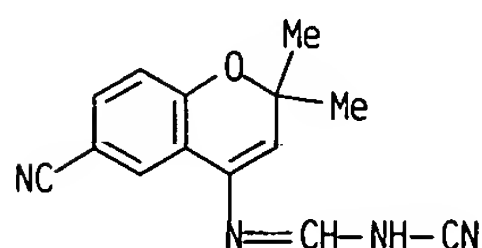
RN 133178-41-3 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



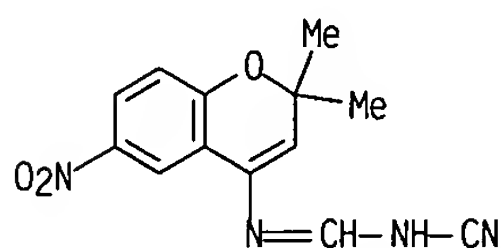
RN 133178-44-6 HCAPLUS

CN Methanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)-
(9CI) (CA INDEX NAME)



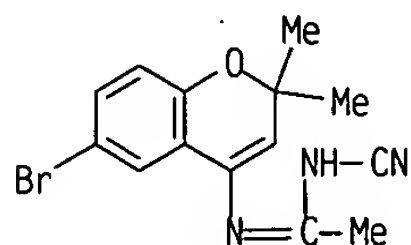
RN 133178-48-0 HCAPLUS

CN Methanimidamide, N-cyano-N'-(2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-
(9CI) (CA INDEX NAME)



RN 133178-50-4 HCAPLUS

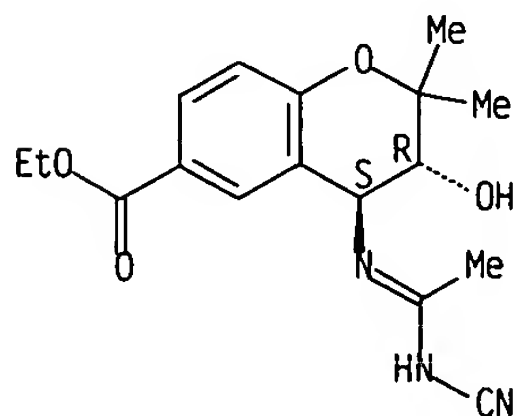
CN Ethanamide, N-(6-bromo-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-
(9CI) (CA INDEX NAME)



RN 133178-55-9 HCAPLUS

CN 2H-1-Benzopyran-6-carboxylic acid, 4-[[1-(cyanoamino)ethylidene]amino]-3,4-dihydro-3-hydroxy-2,2-dimethyl-, ethyl ester, trans- (9CI) (CA INDEX NAME)

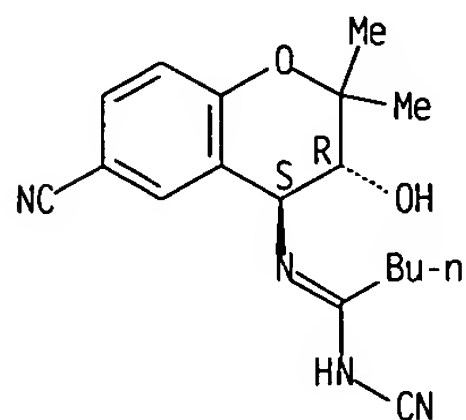
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-45-5 HCAPLUS

CN Pentanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

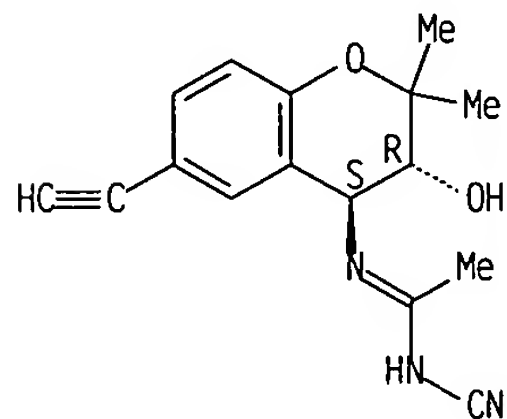
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-49-9 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(6-ethynyl-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

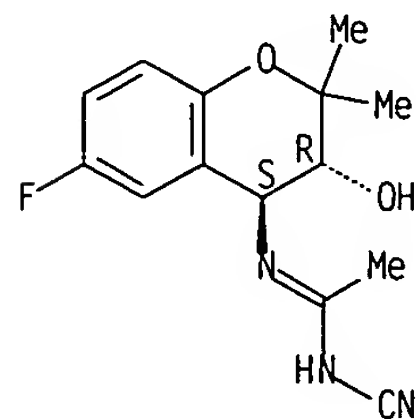
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-52-4 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(6-fluoro-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

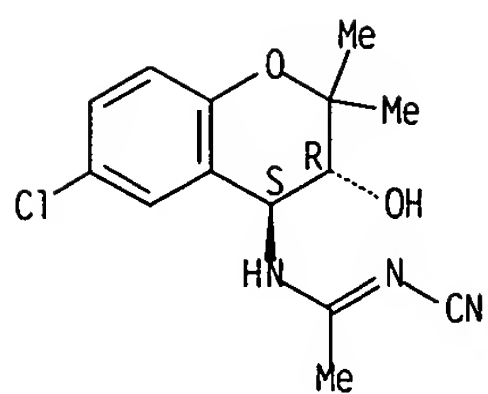
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-53-5 HCAPLUS

CN Ethanimidamide, N-(6-chloro-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

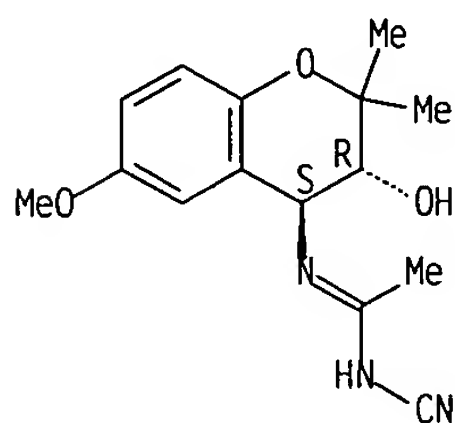
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-54-6 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-6-methoxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

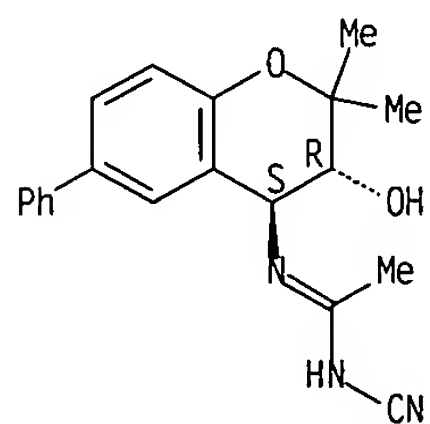
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-55-7 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-phenyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

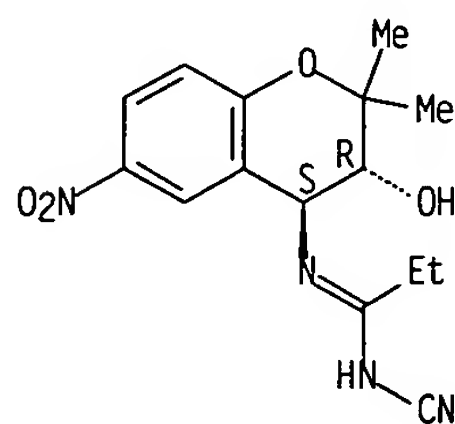
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-56-8 HCAPLUS

CN Propanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

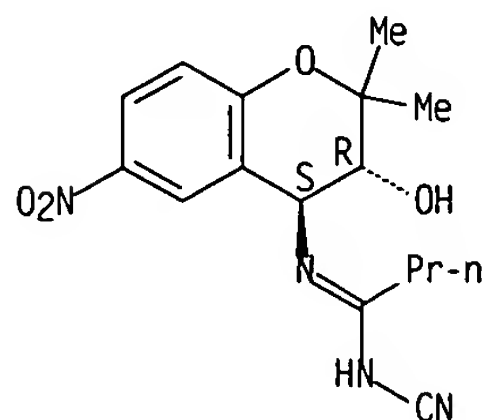
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-57-9 HCAPLUS

CN Butanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

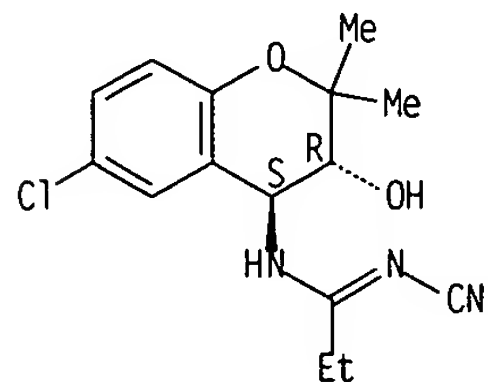
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-58-0 HCAPLUS

CN Propanimidamide, N-(6-chloro-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

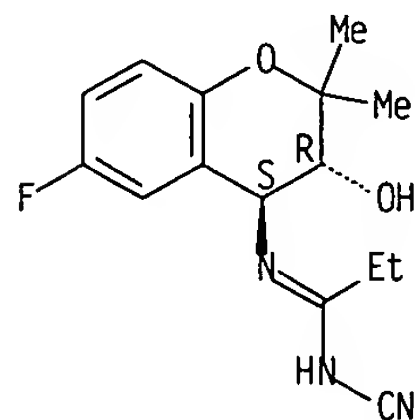
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-59-1 HCAPLUS

CN Propanimidamide, N-cyano-N'-(6-fluoro-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

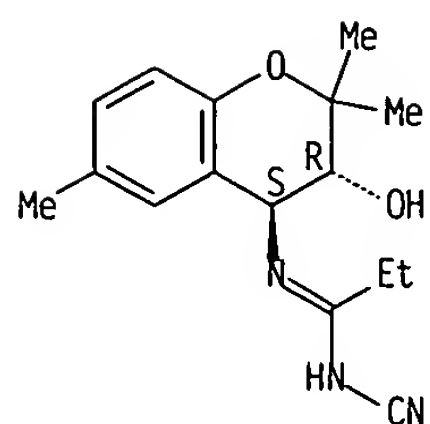
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-60-4 HCAPLUS

CN Propanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2,6-trimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

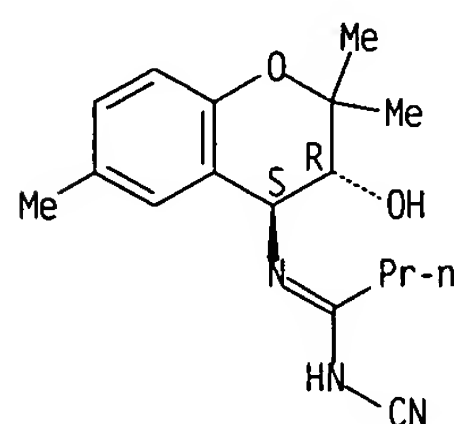
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-61-5 HCAPLUS

CN Butanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2,6-trimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

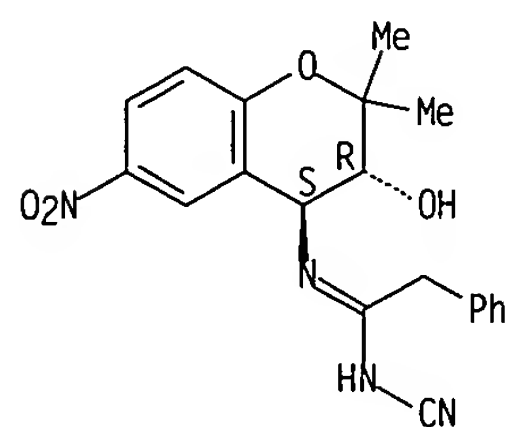
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-62-6 HCAPLUS

CN Benzeneethanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

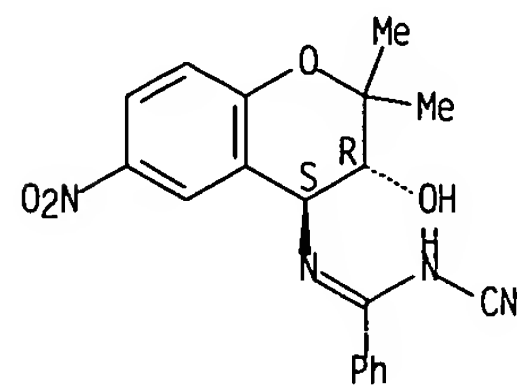
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-63-7 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

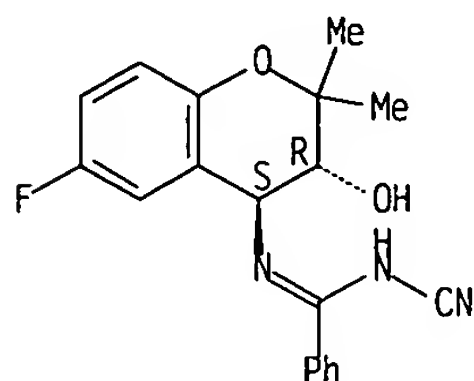
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-64-8 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-fluoro-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

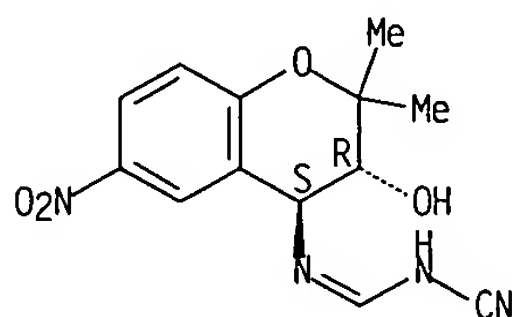
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-65-9 HCAPLUS

CN Methanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

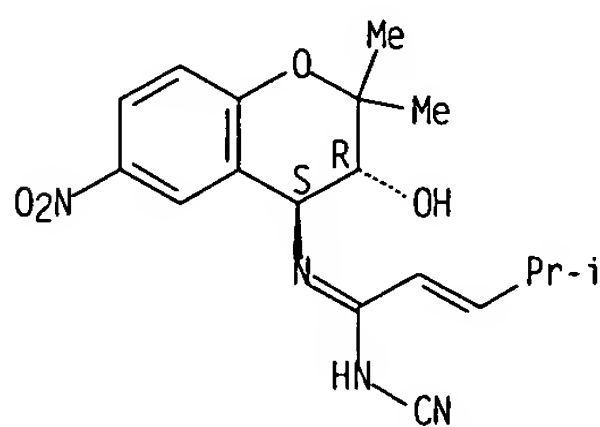
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-66-0 HCAPLUS

CN 2-Pentenimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-4-methyl-, trans- (9CI) (CA INDEX NAME)

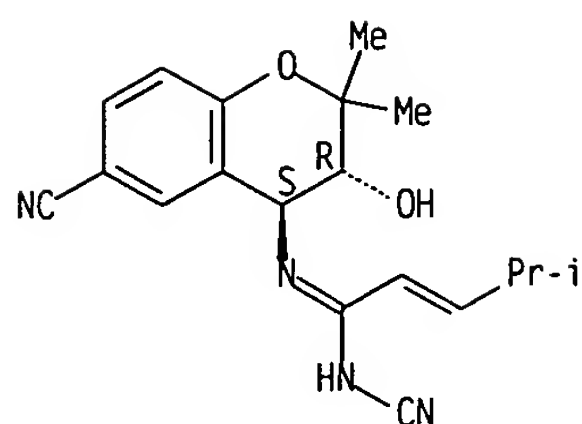
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-67-1 HCAPLUS

CN 2-Pentenimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-4-methyl-, trans- (9CI) (CA INDEX NAME)

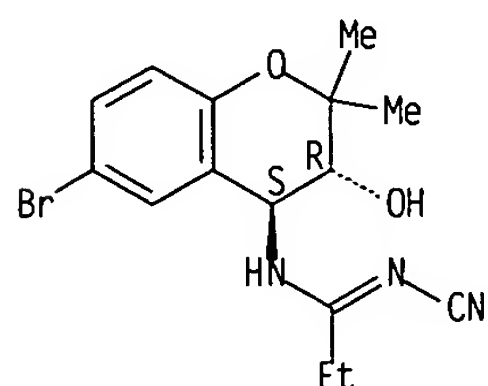
Relative stereochemistry.
Double bond geometry unknown.



RN 134827-68-2 HCAPLUS

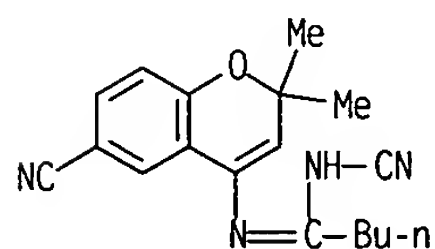
CN Propanimidamide, N-(6-bromo-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



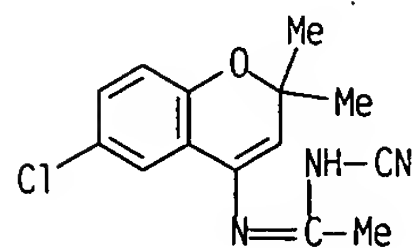
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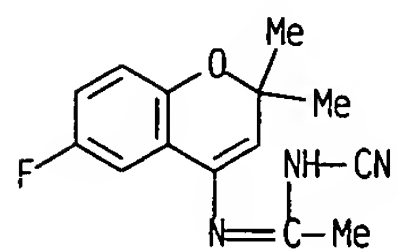
RN 134827-70-6 HCAPLUS

CN Ethanimidamide, N-(6-chloro-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano- (9CI) (CA INDEX NAME)

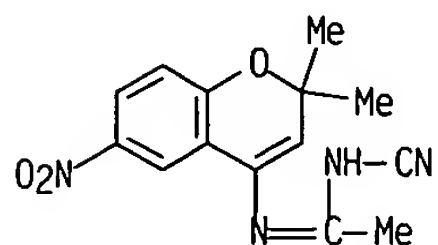


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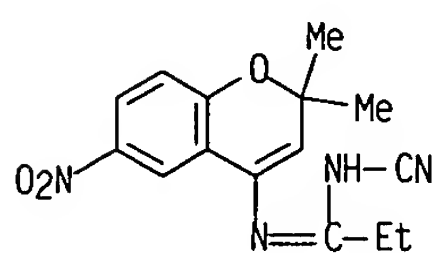
CN Ethanimidamide, N-cyano-N'-(6-fluoro-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



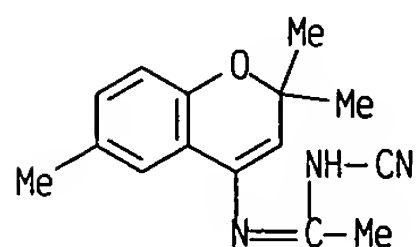
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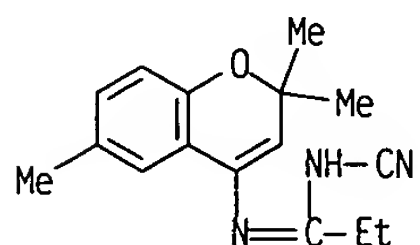
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 CN Propanimidamide, N-cyano-N'-(2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-
 (9CI) (CA INDEX NAME)



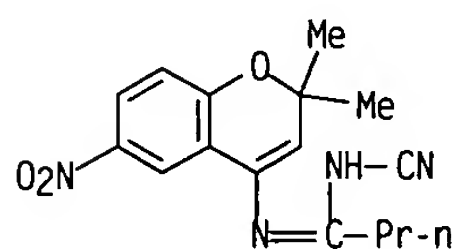
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 CN Ethanimidamide, N-cyano-N'-(2,2,6-trimethyl-2H-1-benzopyran-4-yl)- (9CI)
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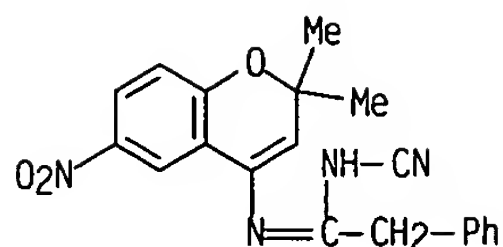
RN 134827-75-1 HCAPLUS
 CN Propanimidamide, N-cyano-N'-(2,2,6-trimethyl-2H-1-benzopyran-4-yl)- (9CI)
 (CA INDEX NAME)



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 (9CI) (CA INDEX NAME)

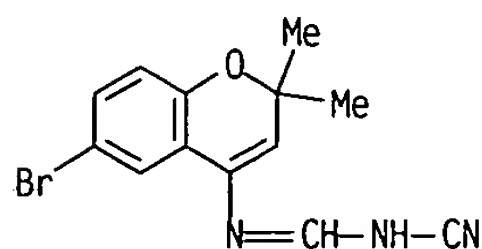


RN 134827-77-3 HCAPLUS
 CN Benzeneethanimidamide, N-cyano-N'-(2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-
 (9CI) (CA INDEX NAME)



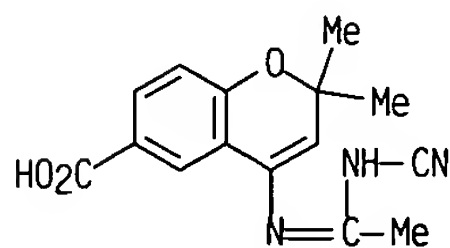
RN 134827-78-4 HCAPLUS

CN Methanimidamide, N-(6-bromo-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano- (9CI) (CA INDEX NAME)



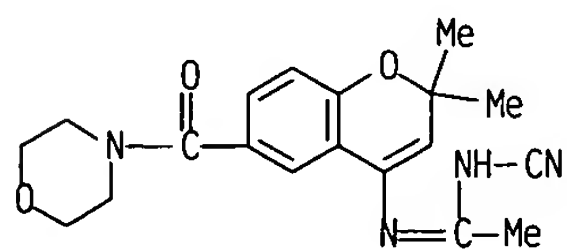
RN 134828-08-3 HCAPLUS

CN 2H-1-Benzopyran-6-carboxylic acid, 4-[[1-(cyanoamino)ethylidene]amino]-2,2-dimethyl- (9CI) (CA INDEX NAME)



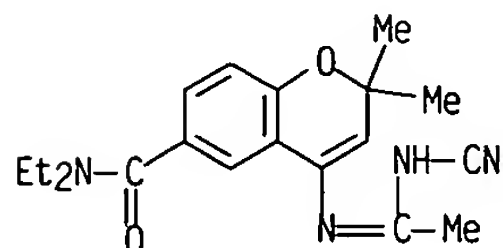
RN 134828-09-4 HCAPLUS

CN Morpholine, 4-[[4-[[1-(cyanoamino)ethylidene]amino]-2,2-dimethyl-2H-1-benzopyran-6-yl]carbonyl]- (9CI) (CA INDEX NAME)



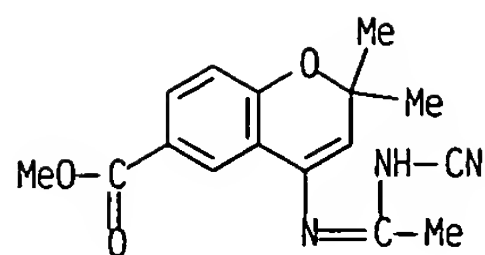
RN 134828-10-7 HCAPLUS

CN 2H-1-Benzopyran-6-carboxamide, 4-[[1-(cyanoamino)ethylidene]amino]-N,N-diethyl-2,2-dimethyl- (9CI) (CA INDEX NAME)



RN 134828-11-8 HCAPLUS

CN 2H-1-Benzopyran-6-carboxylic acid, 4-[[1-(cyanoamino)ethylidene]amino]-2,2-dimethyl-, methyl ester (9CI) (CA INDEX NAME)



L24 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1991:247115 HCAPLUS
 DN 114:247115
 ED Entered STN: 28 Jun 1991
 TI Preparation of N"-cyano-N-(6-cyano-3-hydroxy-3,4-dihydro-2H-1-benzopyran-4-yl)guanidines and analogs as cardiovascular agents
 IN Atwal, Karnail; Grover, Gary James; Kim, Kyoung Soon
 PA E. R. Squibb and Sons, Inc., USA
 SO Eur. Pat. Appl., 34 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07D311-68
 ICS C07D405-04; C07D491-04; A61K031-35; C07D405-14
 CC 27-7 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1

FAN.CNT 5

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | EP 401010 | A2 | 19901205 | EP 1990-305920 | 19900531 <-- |
| | EP 401010 | A3 | 19910502 | | |
| | EP 401010 | B1 | 19960821 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
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| | CA 2015296 | C | 20010807 | | |
| | AU 9054552 | A1 | 19901206 | AU 1990-54552 | 19900430 <-- |
| | AU 633082 | B2 | 19930121 | | |
| | ZA 9003491 | A | 19910227 | ZA 1990-3491 | 19900508 <-- |
| | IL 94326 | A1 | 19951208 | IL 1990-94326 | 19900508 <-- |
| | IN 173988 | A | 19940820 | IN 1990-DE494 | 19900522 <-- |
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| | JP 03027375 | A2 | 19910205 | JP 1990-143243 | 19900530 <-- |
| | HU 55055 | A2 | 19910429 | HU 1990-3271 | 19900530 <-- |
| | HU 207857 | B | 19930628 | | |
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| | CN 1047672 | A | 19901212 | CN 1990-103959 | 19900531 <-- |
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| | PL 166007 | B1 | 19950331 | PL 1990-285415 | 19900531 <-- |
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| | PL 166230 | B1 | 19950428 | PL 1990-290036 | 19900531 <-- |
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| | JP 05239049 | A2 | 19930917 | JP 1991-158327 | 19910628 <-- |
| | IN 178152 | A | 19970308 | IN 1992-DE96 | 19920207 <-- |
| | IN 180495 | A | 19980207 | IN 1992-DE1111 | 19921126 <-- |
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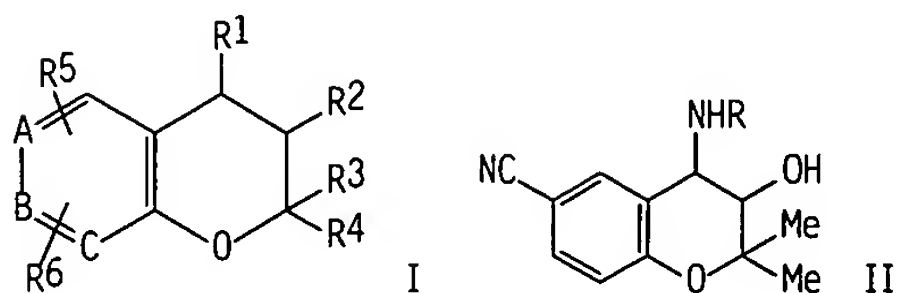
CLASS

PATENT NO. CLASS PATENT FAMILY CLASSIFICATION CODES

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EP 401010      ICM      C07D311-68
                  ICS      C07D405-04; C07D491-04; A61K031-35; C07D405-14
EP 401010      ECLA      C07D311/68; C07D405/04+311+239B; C07D405/06+311+213;
                  C07D491/04+311B+221B; C07F009/655P60; C07F;
                  C07F009/6561; C07F009/6571L4 <--
PL 166174      ECLA      C07F009/655P60; C07F009/6571L4; C07F009/6561;
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PL 166230      ECLA      C07F009/655P60; C07D311/68; C07F009/6561;
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                  C07D311/68; C07D405/04+311+239B <--
OS   MARPAT 114:247115
GI

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AB The title compds. [I; A, B, C = CH or 1 of A, B, C = N or NO and the others = CH; R1 = R7R8NC(:NCN)NR9; R2 = H, OH, OAc; R3, R4 = H, (ar)alkyl; R3 R4 = atoms to form a 5- to 7-membered carbocyclic ring; R5 = H, (halo)alkyl, alkenyl, cyano, etc.; R6 = H, OH, alkoxy, cyano, NO2, (substituted) NH2; R7, R8 = H, (cyclo)alkyl, aryl, heterocyclyl, etc.; NR7R8 = (un)substituted heterocyclyl; R9 = H, (cyclo)alkyl, alkenyl, aryl, etc.; R8R9 = atoms to complete a 5- to 7-membered (un)substituted ring]. K-channel activators, were prepared as antiischemics and antihypertensive (no data). Thus, aminobenzopyran trans-II (R = H) was condensed with NCNHCNHCMe2Et (preparation given) to give trans-II [R = NHC(:NCN)NHCMe2Et].

ST cyanoguanidine cyanohydroxybenzopyranyl prepn cardiovascular;
benzopyranyl cyanoguanidine prepn antiischemic antihypertensive

IT Antihypertensives
(N''-cyano-N-(cyanohydroxydihydrobenzopyranyl)guanidines and analogs)

IT 41835-08-9P 89125-07-5P 118581-55-8P 127419-05-0P 127749-52-4P
129180-58-1P 129180-59-2P 129462-66-4P 130228-87-4P 134017-89-3P
134017-90-6P 134017-91-7P 134017-92-8P 134017-93-9P 134017-94-0P
134017-95-1P 134017-96-2P 134017-97-3P 134017-98-4P 134017-99-5P
134018-00-1P 134018-01-2P 134028-71-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, in preparation of cardiovascular agents)

IT 127249-54-1P 127249-61-0P 127249-68-7P 127249-69-8P 127249-70-1P
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134017-82-6P 134017-83-7P 134017-84-8P 134017-85-9P
134017-86-0P 134017-87-1P 134017-88-2P 134035-97-5P 134053-73-9P
134053-74-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as cardiovascular agent)

IT 75-31-0, Isopropylamine, reactions 100-46-9, Benzylamine, reactions
103-72-0, Phenylisothiocyanate 107-15-3, Ethylenediamine, reactions

109-76-2, 1,3-Diaminopropane 123-75-1, Pyrrolidine, reactions
 536-74-3, Phenylacetylene 540-38-5, 4-Iodophenol 542-85-8, Ethyl
 isothiocyanate 597-97-7 611-71-2, (R)-(-)-Mandelic acid 811-93-8,
 1,1-Dimethylethylenediamine 1111-97-3, 3-Chloro-3-methyl-1-butyne
 2759-28-6 3731-52-0, 3-(Aminomethyl)pyridine 3731-53-1,
 4-(Aminomethyl)pyridine 4788-37-8 10191-60-3 16035-50-0
 17199-29-0, (S)-(+)-Mandelic acid 17292-62-5, Monosodium cyanamide
 65018-90-8 79463-77-7, Diphenylcyanocarbonimidate 86776-58-1
 86823-96-3 89316-91-6 108031-11-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of cardiovascular agents)

IT 7440-09-7, Potassium, biological studies

RL: BPR (Biological process); BIOL (Biological study); PROC (Process)

(transport of, activation of, N''-cyano-N-(cyanohydroxydihydrobenzopyra
 nyl)guanidines and analogs as)

IT 127249-72-3P 134017-82-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);

BIOL (Biological study); PREP (Preparation); USES (Uses)

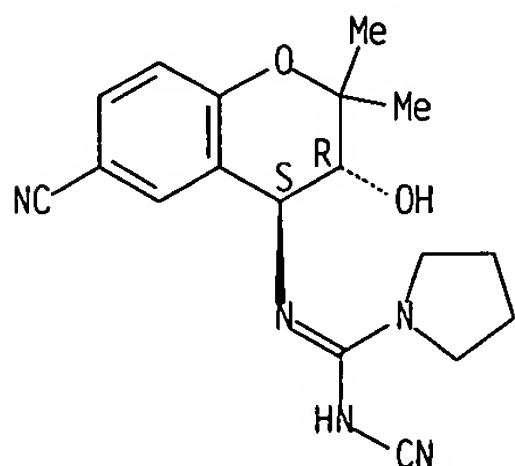
(preparation of, as cardiovascular agent)

RN 127249-72-3 HCAPLUS

CN 1-Pyrrolidinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-
 2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

Double bond geometry unknown.

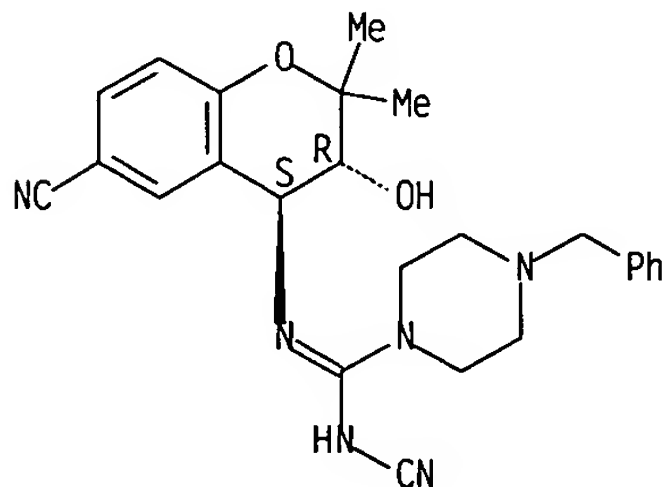


RN 134017-82-6 HCAPLUS

CN 1-Piperazinecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-
 dimethyl-2H-1-benzopyran-4-yl)-4-(phenylmethyl)-, trans- (9CI) (CA INDEX
 NAME)

Relative stereochemistry.

Double bond geometry unknown.



L24 ANSWER 13 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1991:164007 HCAPLUS

DN 114:164007

ED Entered STN: 03 May 1991

TI Preparation of benzopyran derivatives as antihypertensives
 IN Shiokawa, Youichi; Takimoto, Koichi; Takenaka, Kohei; Kato, Takeshi
 PA Fujisawa Pharmaceutical Co., Ltd., Japan
 SO Eur. Pat. Appl., 39 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07D311-68
 ICS C07D405-04; C07D417-04; A61K031-35
 ICI C07D405-04, C07D311-00, C07D207-00; C07D417-04, C07D311-00, C07D277-00
 CC 27-14 (Heterocyclic Compounds (One Hetero Atom))
 Section cross-reference(s): 1

FAN.CNT 1

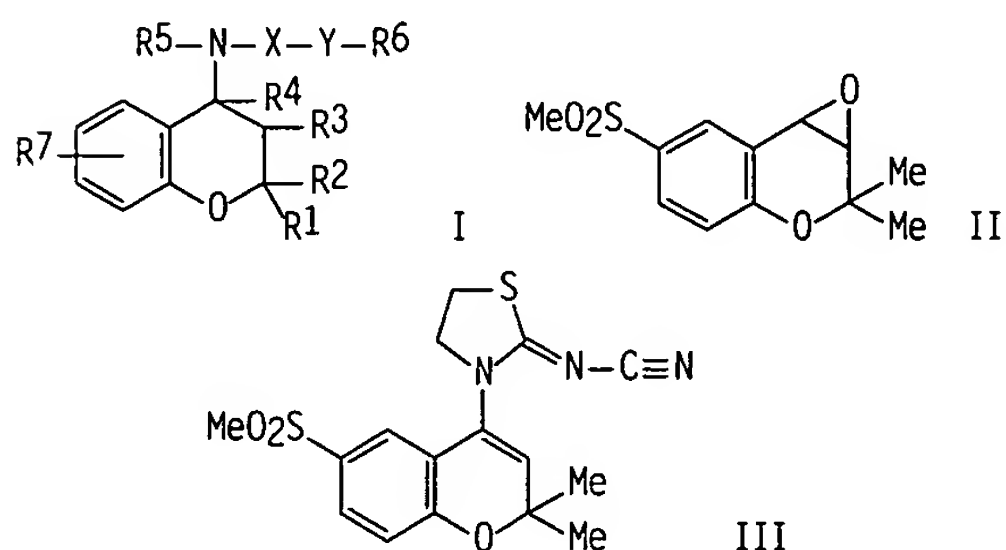
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | EP 389861 | A1 | 19901003 | EP 1990-104702 | 19900313 <-- |
| | EP 389861 | B1 | 19950823 | | |
| | R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | US 5104890 | A | 19920414 | US 1990-490375 | 19900308 <-- |
| | CA 2013163 | AA | 19900928 | CA 1990-2013163 | 19900327 <-- |
| | JP 02300182 | A2 | 19901212 | JP 1990-80045 | 19900328 <-- |
| PRAI | GB 1989-6950 | A | 19890328 | <-- | |
| | GB 1989-9278 | A | 19890424 | <-- | |
| | GB 1989-26822 | A | 19891128 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|--|
| EP 389861 | ICM | C07D311-68 |
| | ICS | C07D405-04; C07D417-04; A61K031-35 |
| | ICI | C07D405-04, C07D311-00, C07D207-00; C07D417-04, C07D311-00, C07D277-00 |
| EP 389861 | ECLA | C07D311/68; C07D405/04+311C+207; C07D417/04+311C+277; C07D417/04+311C+285B; C07D417/04+311C+277B <-- |

OS MARPAT 114:164007

GI



AB Title benzopyrans I [R1,R2 = C1-6 alkyl; R3 = OH or acyloxy and R4 = H, or R3R4 = bond; R5 = H, C1-6 alkyl; R6 = H, C1-6 alkyl, aryl; or R5R6 = alkylene; R7 = cyano, acyl, halo, NO2, C1-6 alkyl, alkylsulfonyl, etc.; X = cyanoiminomethylene or SO2; Y = bond, thio, (C1-6 alkyl)imino] and related compds., useful as antihypertensives, were prepared. For example, reaction of epoxide II (preparation given) with 2-(cyanoimino)thiazolidine at 100.degree. in DMF in the presence of Et2N gave the corresponding I (R3 = OH). Subsequent acetylation and reaction with DBU gave a benzopyran III. III at 1.0 mg/kg i.v. showed a 49.2% maximum decrease in blood pressure in rats.

ST benzopyran prepn antihypertensive; vasodilator benzopyran prepn

IT Antihypertensives

Vasodilators

(benzopyran derivs.)

IT 7440-09-7P. Potassium. preparation
 RL: PREP (Preparation)

(channels, activators for, benzopyran derivs. for)

IT 15020-57-2P, 4-Hydroxy-N,N-dimethylbenzenesulfonamide 19013-07-1P
 59907-37-8P, 4-Methoxy-N,N-dimethylbenzenesulfonamide 65018-69-1P
 65018-70-4P 69964-40-5P 86823-96-3P 89316-91-6P 89316-98-3P
 94470-71-0P 118383-29-2P 118383-30-5P 120728-68-9P 122262-14-0P
 133178-03-7P 133178-61-7P 133178-62-8P 133178-63-9P 133178-64-0P
 133178-65-1P 133178-66-2P 133178-67-3P 133178-68-4P 133178-69-5P
 133946-62-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation and reaction of, in preparation of antihypertensives)

IT 133178-04-8P 133178-05-9P 133178-06-0P 133178-07-1P 133178-08-2P
 133178-09-3P 133178-10-6P 133178-11-7P 133178-12-8P 133178-13-9P
 133178-14-0P 133178-15-1P 133178-16-2P 133178-17-3P 133178-18-4P
 133178-19-5P 133178-20-8P 133178-21-9P 133178-22-0P
 133178-23-1P 133178-24-2P 133178-25-3P
 133178-26-4P 133178-27-5P 133178-28-6P
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 133178-32-2P 133178-33-3P 133178-34-4P
 133178-35-5P 133178-36-6P 133178-37-7P
 133178-38-8P 133178-39-9P 133178-40-2P
 133178-41-3P 133178-42-4P 133178-43-5P
 133178-44-6P 133178-45-7P 133178-46-8P 133178-47-9P
 133178-48-0P 133178-49-1P 133178-50-4P
 133178-51-5P 133178-52-6P 133178-53-7P 133178-54-8P
 133178-55-9P 133178-56-0P 133178-57-1P
 133178-58-2P 133178-59-3P 133178-60-6P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as antihypertensive)

IT 75-16-1, Methylmagnesium bromide 98-68-0, 4-Methoxybenzenesulfonyl
 chloride 124-40-3, Dimethylamine, reactions 1111-97-3,
 3-Chloro-3-methyl-1-butyne 1558-82-3, Ethyl N-cyanoacetimidate
 7664-41-7, Ammonia, reactions 10191-60-3, Dimethyl N-
 cyanoiminodithiocarbonate 26364-65-8, 2-(Cyanoimino)thiazolidine
 33143-29-2 54356-31-9, Ethyl N-cyanopropionimidate 54554-02-8
 67104-97-6 133178-70-8, Methyl N-cyano-4-chlorobutyrimidate
 RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of antihypertensives)

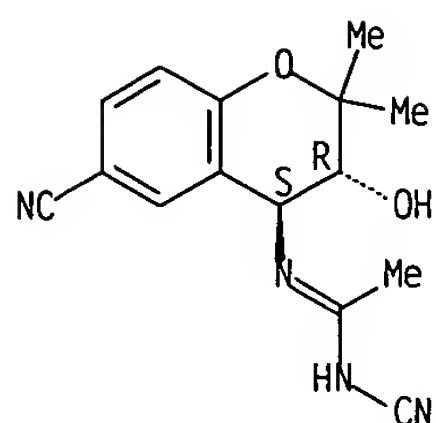
IT 133178-23-1P 133178-24-2P 133178-25-3P
 133178-26-4P 133178-27-5P 133178-28-6P
 133178-29-7P 133178-31-1P 133178-32-2P
 133178-33-3P 133178-34-4P 133178-35-5P
 133178-36-6P 133178-37-7P 133178-38-8P
 133178-39-9P 133178-41-3P 133178-42-4P
 133178-44-6P 133178-47-9P 133178-48-0P
 133178-50-4P 133178-51-5P 133178-53-7P
 133178-55-9P 133178-56-0P 133178-57-1P
 133178-59-3P
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological
 study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
 BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as antihypertensive)

RN 133178-23-1 HCAPLUS

CN Ethanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-
 1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

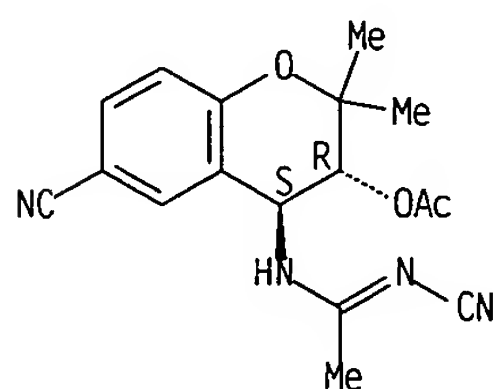
Relative stereochemistry.
 Double bond geometry unknown.



RN 133178-24-2 HCAPLUS

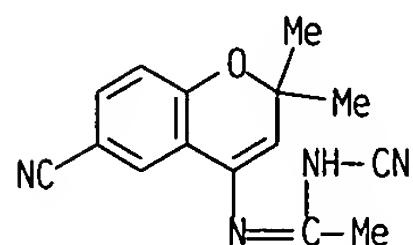
CN Ethanimidamide, N-[3-(acetyloxy)-6-cyano-3,4-dihydro-2,2-dimethyl-2H-1-benzopyran-4-yl]-N'-cyano-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RN 133178-25-3 HCAPLUS

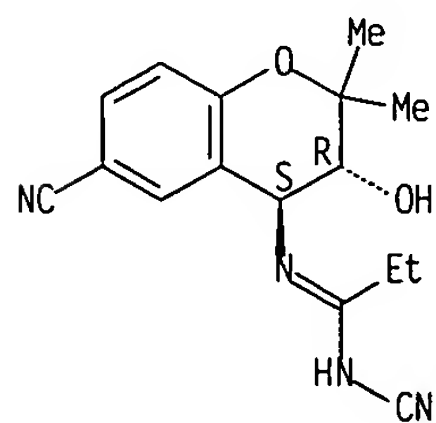
CN Ethanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 133178-26-4 HCAPLUS

CN Propanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

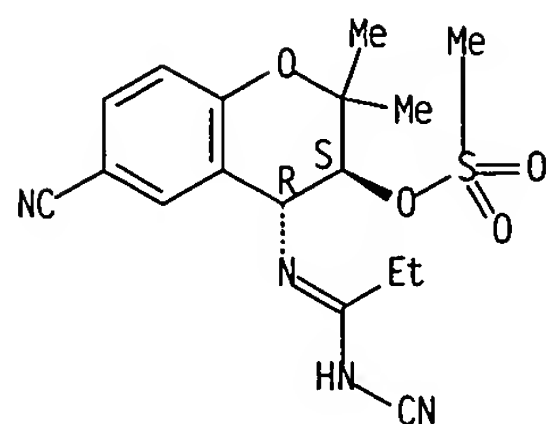


RN 133178-27-5 HCAPLUS

CN Propanimidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2,2-dimethyl-3-[(methylsulfonyl)oxy]-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

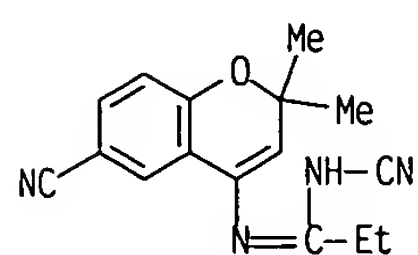
Relative stereochemistry.

Double bond geometry unknown.



RN 133178-28-6 HCAPLUS

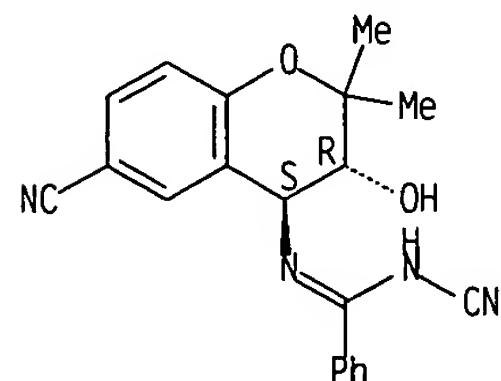
CN Propanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 133178-29-7 HCAPLUS

CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

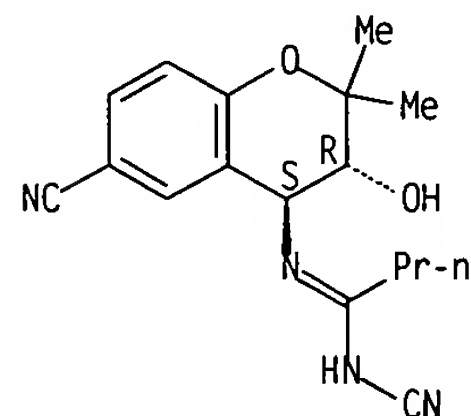
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-31-1 HCAPLUS

CN Butanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

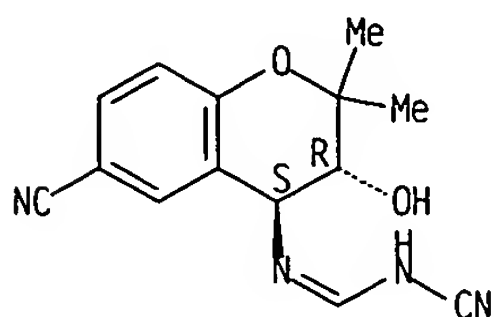
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-32-2 HCAPLUS

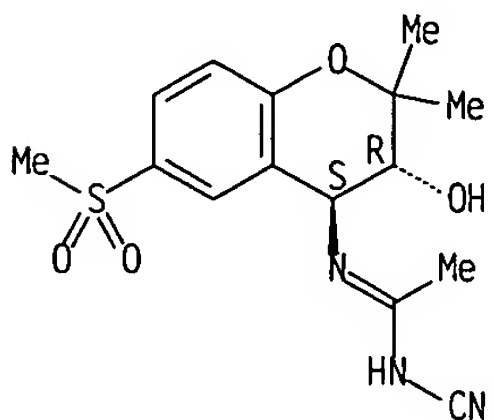
CN Methanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



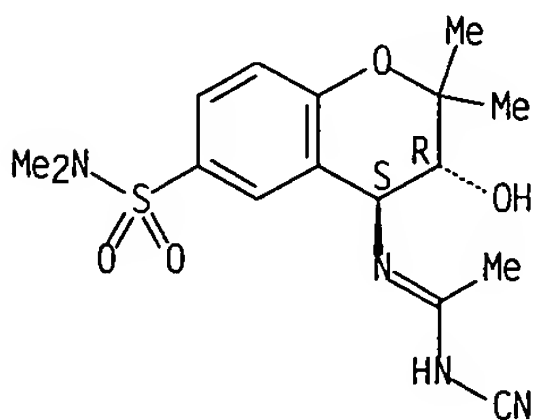
RN 133178-33-3 HCAPLUS
CN Ethanimidamide, N-cyano-N'-[3,4-dihydro-3-hydroxy-2,2-dimethyl-6-(methylsulfonyl)-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



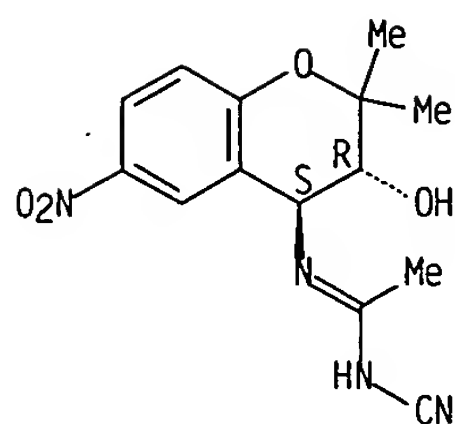
RN 133178-34-4 HCAPLUS
CN Ethanimidamide, N-cyano-N'-[6-[(dimethylamino)sulfonyl]-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RN 133178-35-5 HCAPLUS
CN Ethanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

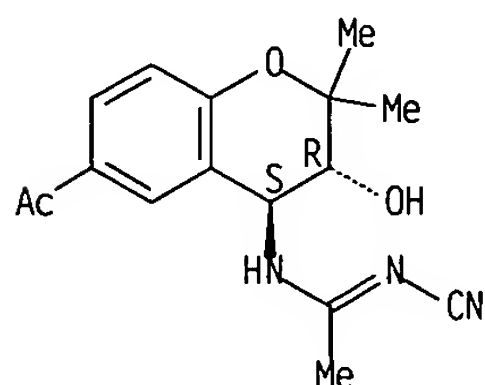
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-36-6 HCAPLUS

CN Ethanimidamide, N-(6-acetyl-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

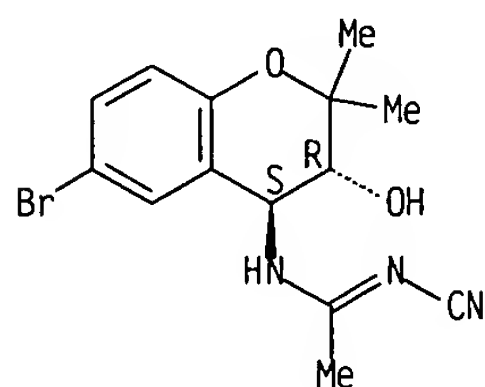
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-37-7 HCAPLUS

CN Ethanimidamide, N-(6-bromo-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano-, trans- (9CI) (CA INDEX NAME)

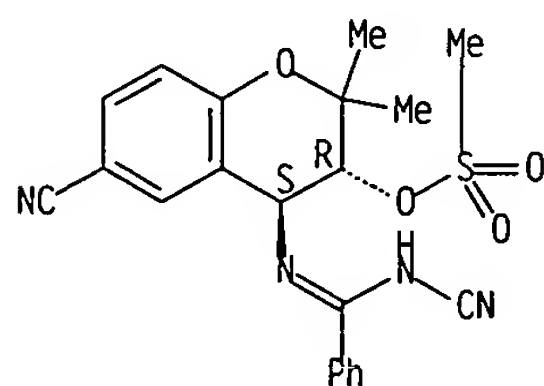
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-38-8 HCAPLUS

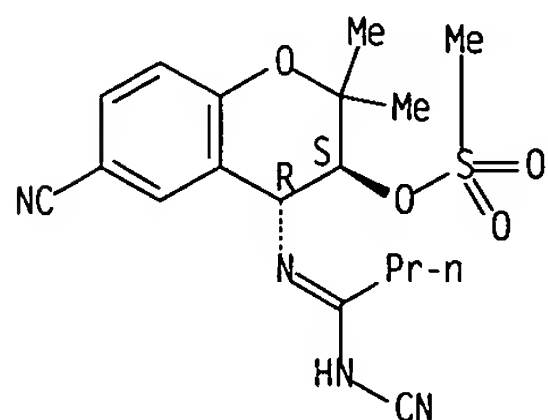
CN Benzenecarboximidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2,2-dimethyl-3-[(methylsulfonyl)oxy]-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

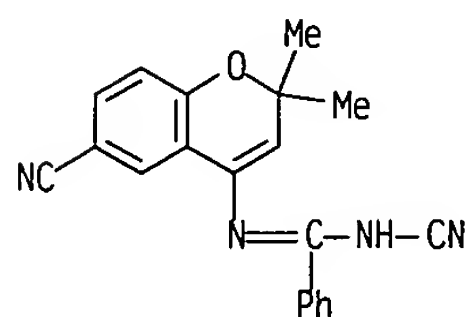


RN 133178-39-9 HCAPLUS
 CN Butanimidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2,2-dimethyl-3-[(methylsulfonyl)oxy]-2H-1-benzopyran-4-yl]-, trans- (9CI) (CA INDEX NAME)

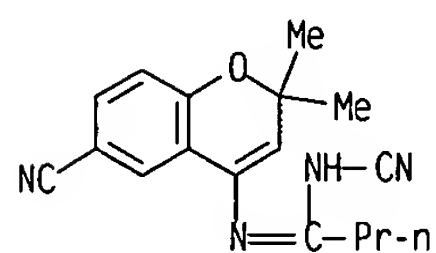
Relative stereochemistry.
 Double bond geometry unknown.



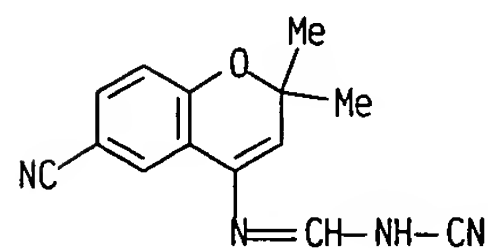
RN 133178-41-3 HCAPLUS
 CN Benzenecarboximidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



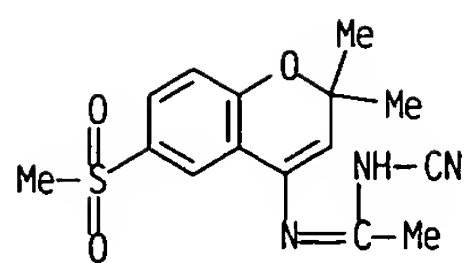
RN 133178-42-4 HCAPLUS
 CN Butanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



RN 133178-44-6 HCAPLUS
 CN Methanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)

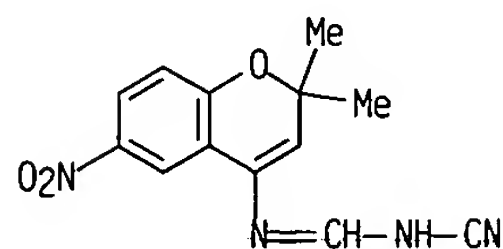


RN 133178-47-9 HCAPLUS
 CN Ethanimidamide, N-cyano-N'-[2,2-dimethyl-6-(methylsulfonyl)-2H-1-benzopyran-4-yl]- (9CI) (CA INDEX NAME)



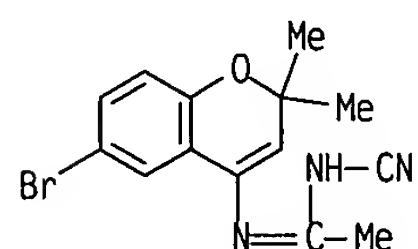
RN 133178-48-0 HCAPLUS

CN Methanimidamide, N-cyano-N'-(2,2-dimethyl-6-nitro-2H-1-benzopyran-4-yl)- (9CI) (CA INDEX NAME)



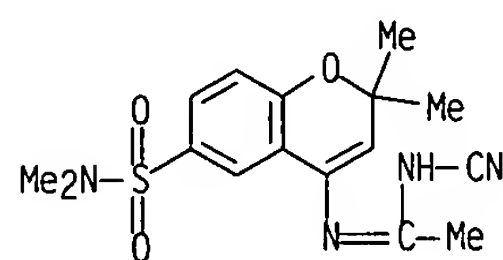
RN 133178-50-4 HCAPLUS

CN Ethanamide, N-(6-bromo-2,2-dimethyl-2H-1-benzopyran-4-yl)-N'-cyano- (9CI) (CA INDEX NAME)



RN 133178-51-5 HCAPLUS

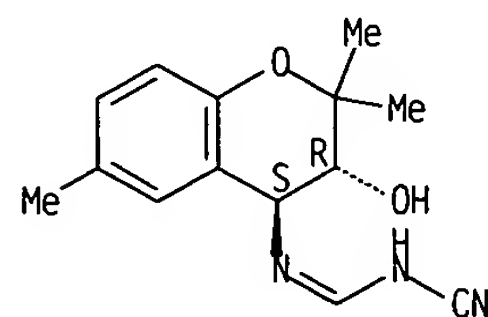
CN Ethanamide, N-cyano-N'-[6-[(dimethylamino)sulfonyl]-2,2-dimethyl-2H-1-benzopyran-4-yl]- (9CI) (CA INDEX NAME)



RN 133178-53-7 HCAPLUS

CN Methanimidamide, N-cyano-N'-(3,4-dihydro-3-hydroxy-2,2,6-trimethyl-2H-1-benzopyran-4-yl)-, trans- (9CI) (CA INDEX NAME)

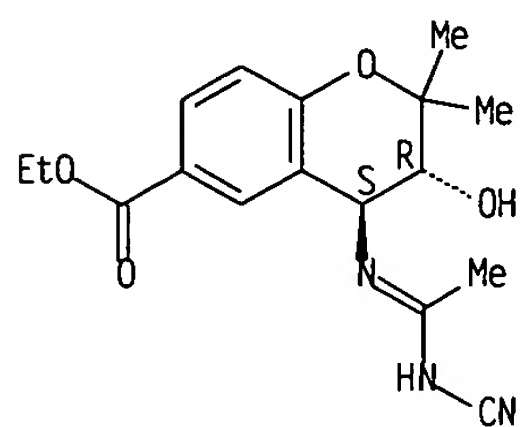
Relative stereochemistry.
Double bond geometry unknown.



RN 133178-55-9 HCAPLUS

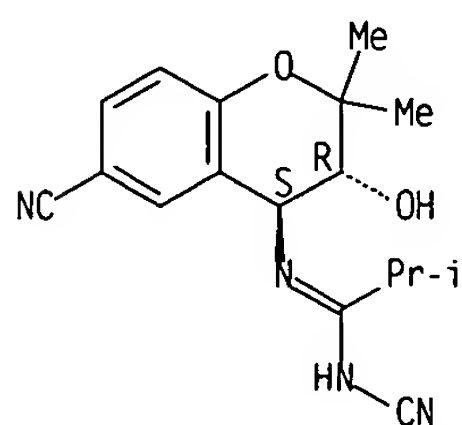
CN 2H-1-Benzopyran-6-carboxylic acid, 4-[[1-(cyanoamino)ethylidene]amino]-3,4-dihydro-3-hydroxy-2,2-dimethyl-, ethyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



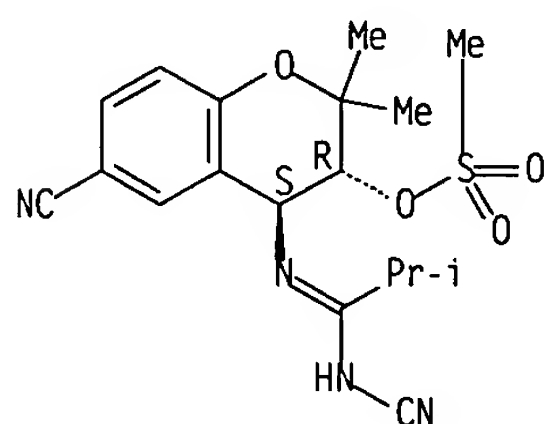
RN 133178-56-0 HCAPLUS
CN Propanimidamide, N-cyano-N'-(6-cyano-3,4-dihydro-3-hydroxy-2,2-dimethyl-2H-1-benzopyran-4-yl)-2-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.

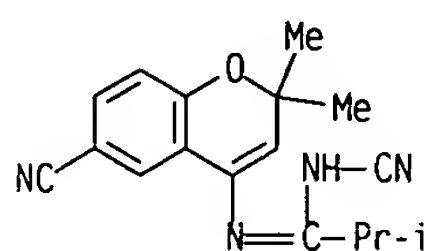


RN 133178-57-1 HCAPLUS
CN Propanimidamide, N-cyano-N'-[6-cyano-3,4-dihydro-2,2-dimethyl-3-[(methylsulfonyl)oxy]-2H-1-benzopyran-4-yl]-2-methyl-, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.
Double bond geometry unknown.



RN 133178-59-3 HCAPLUS
CN Propanimidamide, N-cyano-N'-(6-cyano-2,2-dimethyl-2H-1-benzopyran-4-yl)-2-methyl- (9CI) (CA INDEX NAME)



L24 ANSWER 14 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1990:216931 HCAPLUS
 DN 112:216931
 ED Entered STN: 09 Jun 1990
 TI Imidazolylcyclopentathiophenes as herbicides
 IN Schneider, Hans Dieter
 PA Ciba-Geigy A.-G., Switz.
 SO Eur. Pat. Appl., 60 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 IC ICM C07D409-04
 ICS A01N043-50; C07D333-78; A01N043-12
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5
 FAN.CNT 1

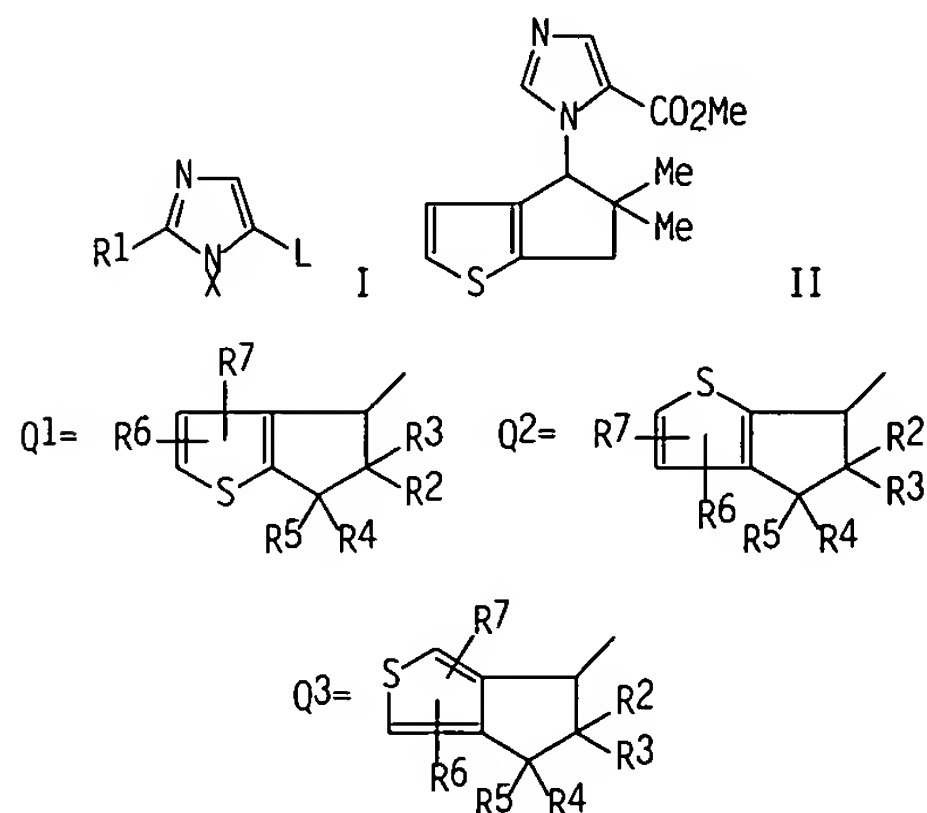
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | EP 347378 | A1 | 19891220 | EP 1989-810423 | 19890605 <-- |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | US 4992090 | A | 19910212 | US 1989-361088 | 19890605 <-- |
| | ZA 8904414 | A | 19900228 | ZA 1989-4414 | 19890612 <-- |
| | JP 02042077 | A2 | 19900213 | JP 1989-150331 | 19890613 <-- |
| PRAI | CH 1988-2251 | A | 19880613 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|------------------------------------|
| EP 347378 | ICM | C07D409-04 |
| | ICS | A01N043-50; C07D333-78; A01N043-12 |

OS MARPAT 112:216931

GI



AB The title compds. (I; X = Q1-Q3; R1 = H, SH; L = cyano, CO₂H, CH₂OH, alkoxycarbonyl, carbamoyl, oximino, etc.; R2, R3 = H, alkyl, alkenyl, alkynyl, R₂R₃ = alkylene; R4, R5 = H, alkyl; R6 = H, cyano, halo, alkyl, haloalkyl, NO₂; R7 = H, halo, alkyl) were prepared Thus, N-cyano-N'-(5,6-dihydro-5,5-dimethyl-4H-cyclopenta[b]thiophen-2-yl)formamidine (prepn given) was stirred 15 h with KOCMe₃ in Me₂SO at room temperature BrCH₂CO₂Me was added and the mixture was stirred 2 h to give the N'-methoxycarbonylmethylformamidine. The latter was refluxed 16 h with

30% NaOMe in MeOH to give Me 4-amino-1-(5,6-dihydro-5,5-dimethyl-4H-cyclopenta[b]thiophen-4-yl)-5-imidazolecarboxylate. The latter was stirred 16 h with Me₃CONO to give imidazole II. II at 4 kg/ha postemergent gave complete control of Avera and Lolium.

ST imidazolylcyclopentathiophene prepn herbicide; cyclopentathiophene imidazolyl prepn herbicide

IT Herbicides
(imidazolylcyclopentathiophenes)

IT 4428-98-2
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminocyclopentathiophene derivative)

IT 96-32-2. Methyl bromoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with thienylcyanoformamide)

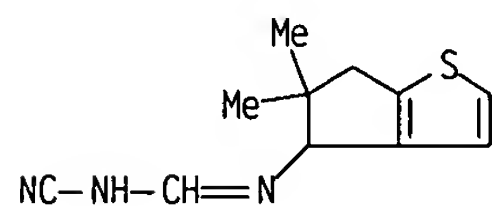
IT 127080-25-5P 127080-26-6P 127080-27-7P 127080-28-8P 127080-29-9P
127080-30-2P 127080-31-3P 127101-99-9P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of, as herbicide)

IT 13196-30-0P 14185-76-3P 26554-84-7P 127080-32-4P 127080-33-5P
127080-34-6P 127080-35-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as herbicide intermediate)

IT 127080-35-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as herbicide intermediate)

RN 127080-35-7 HCAPLUS

CN Methanimidamide, N-cyano-N'-(5,6-dihydro-5,5-dimethyl-4H-cyclopenta[b]thien-4-yl)- (9CI) (CA INDEX NAME)



L24 ANSWER 15 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:632817 HCAPLUS

DN 111:232817

ED Entered STN: 23 Dec 1989

TI Preparation of 1-substituted imidazole-5-carboxylates as herbicides and plant growth regulators

IN Toepfl. Werner

PA Ciba-Geigy A.-G., Switz.

SO Eur. Pat. Appl., 62 pp.
CODEN: EPXXDW

DT Patent

LA German

IC ICM C07D233-90
ICS C07D409-04; C07D405-04; C07D401-04; A01N043-50; A01N043-16;
A01N043-10; A01N043-08; A01N043-42

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
Section cross-reference(s): 5

FAN.CNT 1

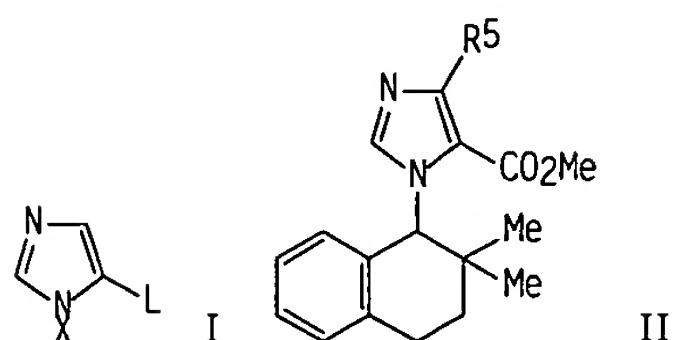
| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|--------------|
| PI | EP 314852 | A2 | 19890510 | EP 1987-810755 | 19871214 <-- |
| | EP 314852 | A3 | 19900418 | | |
| | EP 314852 | B1 | 19931118 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | IL 84809 | A1 | 19921201 | IL 1987-84809 | 19871214 <-- |

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| AU 8782554 | A1 | 19890511 | AU 1987-82554 | 19871215 <-- |
| AU 606907 | B2 | 19910221 | | |
| ZA 8709396 | A | 19890726 | ZA 1987-9396 | 19871215 <-- |
| CA 1294612 | A1 | 19920121 | CA 1987-554454 | 19871216 <-- |
| BR 8706929 | A | 19890718 | BR 1987-6929 | 19871218 <-- |
| US 4921955 | A | 19900501 | US 1987-136167 | 19871218 <-- |
| JP 01135772 | A2 | 19890529 | JP 1987-322626 | 19871219 <-- |
| PRAI CH 1987-4331 | A | 19871106 | <-- | |

CLASS

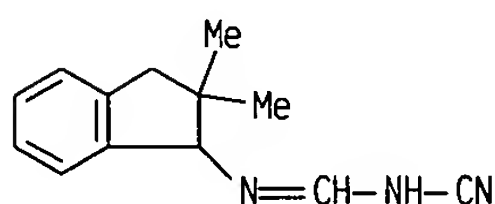
| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|---|
| EP 314852 | ICM | C07D233-90 |
| | ICS | C07D409-04; C07D405-04; C07D401-04; A01N043-50; A01N043-16; A01N043-10; A01N043-08; A01N043-42 |

GI

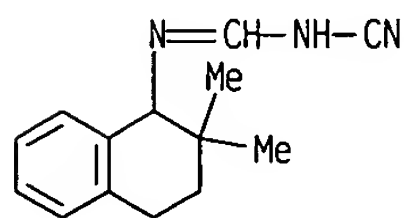


- AB The title compds. [I; L = CO₂R₁, CONR₂R₃, CONR₄NHR₃, CN, etc., X = (substituted) 1-indanyl, 1-tetrahydronaphtholyl, 5-benzocycloheptenyl, 4-tetrahydrobenzothienyl, 4-tetrahydrobenzofuryl, 5-tetrahydroquinolyl, 9,10-dihydro-9-anthracenyl, 9H-fluoren-9-yl, 5-dibenzo[a,d]cycloheptenyl, 1-dihydronaphthalinyl, etc.; R₁ = H, C1-7 alkyl, C3-7 alkenyl, alkynyl, cycloalkyl, alkoxyalkyl, arylalkyl; R₂-R₄ = H, C1-5 alkyl, C3-5 alkenyl, alkynyl, C3-7 cycloalkoxyl, aryl, etc.; R₂R₃N = (substituted) piperidinyl, pyrrolidinyl, 2-oxopiperidinyl, 2-oxopyrrolidinyl, morpholinyl, thiomorpholino, piperazinyl, alkyl piperazinyl], useful as herbicides and plant growth regulators (no data), were prepared MeOCOCH₂N(Q)CH:NCN (Q = 2,2-dimethyl-1,2,3,4-tetrahydronaphth-1-yl) (preparation given) in MeOH was refluxed with NaOMe for 2 h to give 4-aminoimidazole II (R₅ = NH₂). The latter in HOAc/HOAcEt was treated with H₃PO₄ and NaNO₂ at 0.degree. to give a diazonium salt solution, which was treated with H₃PO₂ to give II (R₅ = H).
- ST arylimidazolecarboxylate prepn herbicide; imidazolecarboxylate aryl prepn herbicide; plant growth regulator arylimidazolecarboxylate prepn
- IT Herbicides
(arylimidazolecarboxylates)
- IT Plant hormones and regulators
RL: RCT (Reactant); RACT (Reactant or reagent)
(arylimidazolecarboxylates)
- IT 4428-98-2, Ethoxymethylenecyanamide
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with aminotetrahydronaphthalene derivative, in preparation of agrochem.)
- IT 96-32-2, Methyl bromoacetate
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with arylaminomethylenecyanamide, in preparation of agrochem.)
- IT 87-62-7, 2,6-Dimethylaniline 91-00-9, Diphenylmethylaniline 110324-26-0
119084-51-4 123981-65-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(condensation of, with ethoxymethylenecyanamide, in preparation of agrochem.)

IT 18391-58-7P 18438-41-0P 69840-18-2P 88490-47-5P 88490-49-7P
 101976-67-4P 110323-21-2P 110323-47-2P 110323-50-7P 110323-68-7P
 110323-73-4P 110323-75-6P 110323-95-0P 110323-97-2P 110324-02-2P
 110324-04-4P 119293-81-1P 119293-82-2P 119293-83-3P 119293-86-6P
 123981-29-3P 123981-31-7P 123981-32-8P 123981-33-9P 123981-34-0P
 123981-35-1P 124000-03-9P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as herbicide and plant growth regulator)
 IT 105364-24-7P 119084-54-7P 123981-36-2P 123981-37-3P
 123981-38-4P 123981-39-5P 123981-40-8P 123981-41-9P
 123981-42-0P 123981-43-1P 123981-44-2P 123981-45-3P 123981-46-4P
 123981-47-5P 123981-48-6P 123981-49-7P 123981-50-0P 123981-51-1P
 123981-52-2P 123981-53-3P 123981-54-4P 123981-55-5P 123981-56-6P
 123981-57-7P 123981-58-8P 123981-59-9P 123981-61-3P 123981-63-5P
 123981-64-6P 123995-90-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for herbicide and plant growth regulator)
 IT 123981-66-8
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of arylimidazolecarboxylate agrochem.)
 IT 119084-54-7P 123981-36-2P 123981-38-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for herbicide and plant growth regulator)
 RN 119084-54-7 HCAPLUS
 CN Methanimidamide, N-cyano-N'-(2,3-dihydro-2,2-dimethyl-1H-inden-1-yl)-
 (9CI) (CA INDEX NAME)

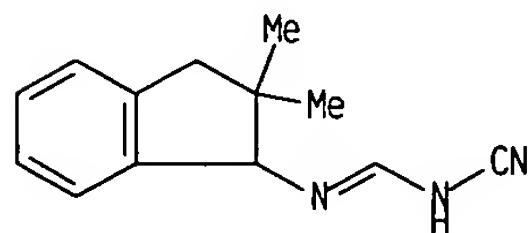


RN 123981-36-2 HCAPLUS
 CN Methanimidamide, N-cyano-N'-(1,2,3,4-tetrahydro-2,2-dimethyl-1-naphthalenyl)- (9CI) (CA INDEX NAME)



RN 123981-38-4 HCAPLUS
 CN Methanimidamide, N-cyano-N'-(2,3-dihydro-2,2-dimethyl-1H-inden-1-yl)-, (+)- (9CI) (CA INDEX NAME)

Rotation (+).
 Double bond geometry unknown.



L24 ANSWER 16 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1989:594762 HCAPLUS

DN 111:194762
 ED Entered STN: 25 Nov 1989
 TI Preparation of imidazole derivatives as herbicides
 IN Schneider, Hans Dieter; Lutz, William R.; Szczepanski, Henry; Topfl, Werner
 PA Ciba-Geigy A.-G., Switz.: Janssen Pharmaceutica N. V.
 SO Eur. Pat. Appl., 42 pp.
 CODEN: EPXXDW
 DT Patent
 LA German
 IC ICM C07D405-04
 ICS C07D409-04; C07D401-04; C07D217-24; C07D221-20; C07D311-76;
 C07D311-96; C07D335-06; C07D335-04
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5

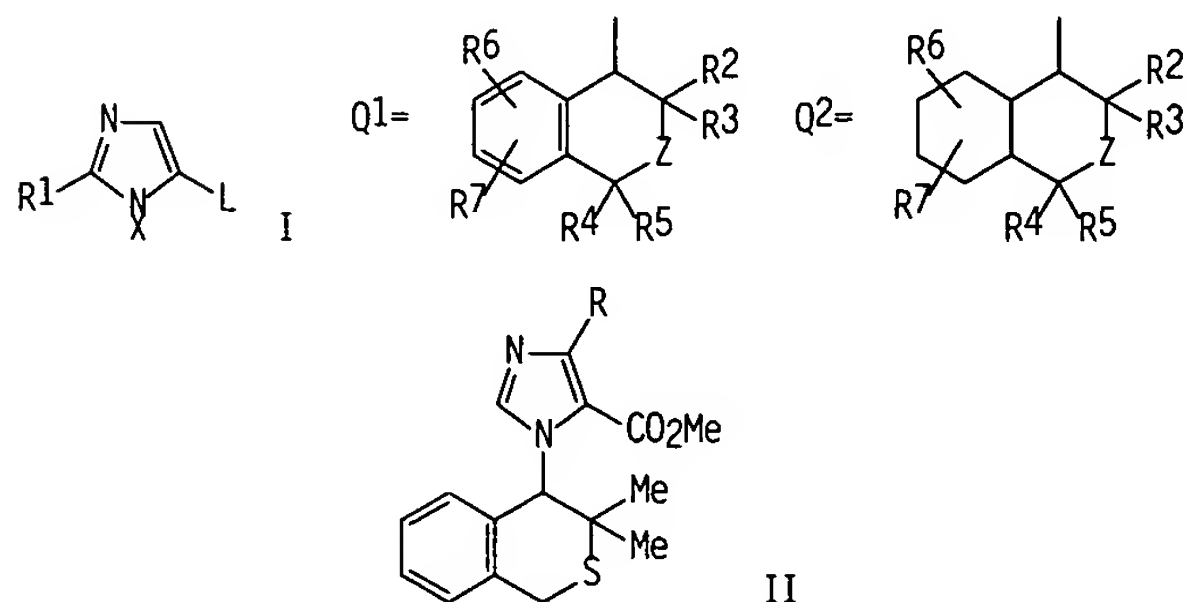
FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------|---|------|----------|-----------------|--------------|
| PI | EP 305332 | A2 | 19890301 | EP 1988-810562 | 19880817 <-- |
| | EP 305332 | A3 | 19900404 | | |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | US 4904300 | A | 19900227 | US 1988-233299 | 19880817 <-- |
| | ZA 8806310 | A | 19890530 | ZA 1988-6310 | 19880825 <-- |
| | JP 01121286 | A2 | 19890512 | JP 1988-212282 | 19880826 <-- |
| PRAI | CH 1987-3262 | A | 19870826 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|---|
| EP 305332 | ICM | C07D405-04 |
| | ICS | C07D409-04; C07D401-04; C07D217-24; C07D221-20; C07D311-76; C07D311-96; C07D335-06; C07D335-04 |

GI



AB The title compds. [I; R1 = H, SH; L = cyano, CO2R8, CONR9R10, etc.; X = heterocyclyl group Q1, Q2; R2, R3 = H, alkyl, alkenyl, alkynyl; R2R3 = alkylene; R4, R5 = H, alkyl; R4R5 = O; R6 = H, alkoxy, halo, alkyl; R7 = H, alkoxy, halo, alkyl, cyano, haloalkyl, haloalkoxy, (halo)alkylthio, NO2; R8 = alkyl, cycloalkyl, alkoxyalkyl, PhCH2, etc.; R9 = H, alkyl, alkoxy, Ph, PhCH2, etc.; R10 = H, alkyl; NR9R10 = pyrrolidino, piperidino, morpholino; Z = O, S, SO, SO2, NR14; R14 = H, alkyl, alkanoyl, alkoxy carbonyl, CO2CH2Ph, Bz, PhCH2] were prepared QNH2 (Q = Q1, R2 = R3 = Me, R4-R7 = H, Z = S) (preparation given) was stirred 2 h with EtOCH:NCN to give QNHCH:NCN which was stirred 2 h with KOCHMe3 in DMSO, followed by addition of BrCH2CO2Me and 16 h stirring, to give NCN:CHNQCH2CO2Me. The latter was refluxed 16 h with NaOMe in MeOH to give

isothiochromanylimidazolecarboxylate II (R = NH₂) which was diazotized and hydrolyzed to give II (R = H) which gave complete control of *Echinochloa crus galli* and *Monarcharia vaginalis* at 4 kg/ha.

ST imidazole deriv prepn herbicide

IT Cereal

Corn

Rice

(herbicides for. imidazole derivs. as)

IT Herbicides

(imidazole derivs.)

IT 123470-03-1P 123470-04-2P 123470-05-3P 123470-06-4P

123470-16-6P 123470-17-7P 123470-18-8P 123470-19-9P 123490-68-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of. in preparation of herbicides)

IT 123469-95-4P 123469-96-5P 123469-97-6P 123469-98-7P 123469-99-8P

123470-00-8P 123470-01-9P 123470-02-0P 123470-07-5P 123470-08-6P

123470-09-7P 123470-10-0P 123470-11-1P 123470-12-2P 123470-13-3P

123470-14-4P 123470-15-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as herbicide)

IT 96-32-2. Methylbromoacetate 4428-98-2 16994-33-5, 3,3-

Dimethylisothiochroman-4-one

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of herbicides)

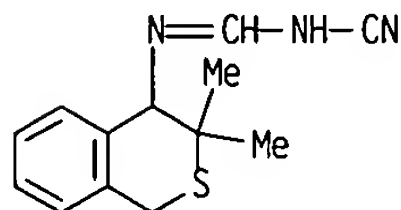
IT 123470-04-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of. in preparation of herbicides)

RN 123470-04-2 HCAPLUS

CN Methanimidamide, N-cyano-N'-(3,4-dihydro-3,3-dimethyl-1H-2-benzothiopyran-4-yl)- (9CI) (CA INDEX NAME)



L24 ANSWER 17 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN

AN 1989:95241 HCAPLUS

DN 110:95241

ED Entered STN: 17 Mar 1989

TI Preparation and testing of 1,5-disubstituted 1H-imidazoles as herbicides

IN De Bruyn, Marcel Frans Leopold; Van Lommen, Guy Rosalia Eugene; Lutz, William R.

PA Janssen Pharmaceutica N. V., Belg.; Ciba-Geigy A.-G.

SO Eur. Pat. Appl., 54 pp.

CODEN: EPXXDW

DT Patent

LA English

IC ICM C07D233-84

ICS C07D233-60; C07D233-61; C07D401-06; C07D405-04; C07D405-14;

C07D409-04; C07D401-04; A01N043-50; A01N043-36; A01N043-16

CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))

Section cross-reference(s): 5

FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|------------|------|----------|-----------------|--------------|
| PI | EP 289066 | A1 | 19881102 | EP 1988-200586 | 19880329 <-- |

R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE

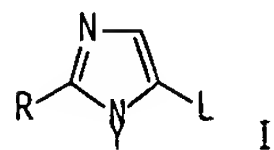
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|-------------------|----|----------|----------------|--------------|
| US 4878940 | A | 19891107 | US 1988-173511 | 19880325 <-- |
| AU 8813846 | A1 | 19881006 | AU 1988-13846 | 19880329 <-- |
| AU 598652 | B2 | 19900628 | | |
| DK 8801798 | A | 19881003 | DK 1988-1798 | 19880330 <-- |
| ZA 8802346 | A | 19891227 | ZA 1988-2346 | 19880331 <-- |
| JP 01019070 | A2 | 19890123 | JP 1988-78301 | 19880401 <-- |
| US 4994103 | A | 19910219 | US 1989-420248 | 19891012 <-- |
| PRAI GB 1987-7856 | A | 19870402 | <-- | |
| GB 1987-29798 | A | 19871222 | <-- | |
| US 1988-173511 | A3 | 19880325 | <-- | |

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|--|
| EP 289066 | ICM | C07D233-84 |
| | ICS | C07D233-60; C07D233-61; C07D401-06; C07D405-04; C07D405-14; C07D409-04; C07D401-04; A01N043-50; A01N043-36; A01N043-16 |

OS MARPAT 110:95241

GI



AB The title compds. [I: R = H, SH; L = C(:X)R1, CR1(ZR2)2, etc.; X = NH, O, S; R1 = H, C1-7 alkyl, C3-7 cycloalkyl, fluoroalkyl, aralkyl, aryl; R2 = (substituted) C1-5 alkyl, C5-7 cycloalkyl, C1-5 alkoxy, alkylthio, halo; R22 = (substituted) CH2CH2, CH2CH2CH2; Y = 1-indanyl, tetrahydro-1-naphthalenyl, benzocyclohepten-5-yl, tetrahydro-4-benzothienyl, etc.], useful as herbicides, were prepared N-(2-Oxo-2-phenylethyl)-N-(1,2,3,4-tetrahydro-1-naphthalenyl)formamide in THF was treated with NaH in THF; after 20 min MeO2CH was added and the mixture was stirred overnight. The product was stirred with KSCN/HCl/MeOH/H2O to give 11.3% [2-mercapto-1-(1,2,3,4-tetrahydro-1-naphthalenyl)-1H-imidazol-5-yl]phenylmethanone. The latter was stirred in a 1:1 mixture of H2O/concentrate HNO3 at 50.degree. for 30 min to give 8.4% phenyl[1-(1,2,3,4-tetrahydro-1-naphthalenyl)-1H-imidazol-5-yl]methanone-HNO3. At 4 kg/ha preemergent I gave complete control of Echinochloa crus-galli while leaving maize unaffected.

ST imidazole disubstituted prepn herbicide

IT Corn

Rice

(herbicides for, imidazole derivs. as)

IT Herbicides

(imidazole derivs.)

IT 110323-21-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(Grignard reaction of, in preparation of herbicide)

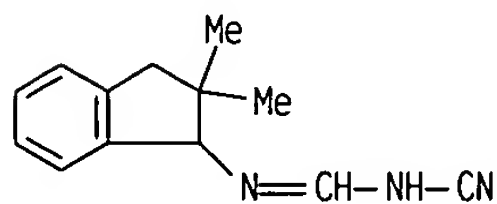
IT 4428-98-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(condensation of, with dimethylindanamine, in preparation of herbicide)

| | | | | |
|-----------------|--------------|--------------|--------------|--------------|
| IT 118259-95-3P | 118259-96-4P | 119084-30-9P | 119084-31-0P | 119084-32-1P |
| 119084-34-3P | 119084-35-4P | 119084-36-5P | 119084-37-6P | 119084-39-8P |
| 119084-40-1P | 119084-41-2P | 119084-42-3P | 119084-43-4P | 119084-44-5P |
| 119084-45-6P | 119084-46-7P | 119084-47-8P | 119084-48-9P | 119084-49-0P |
| 119084-56-9P | 119084-57-0P | 119084-58-1P | 119084-59-2P | 119084-60-5P |
| 119084-61-6P | 119084-62-7P | 119084-63-8P | 119084-64-9P | 119084-65-0P |
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| 119084-79-6P | 119084-81-0P | 119084-82-1P | 119084-83-2P | 119084-85-4P |

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 119084-92-3P 119084-94-5P 119084-95-6P 119084-97-8P 119084-99-0P
 119085-01-7P 119085-02-8P 119085-03-9P 119085-04-0P 119085-05-1P
 119085-06-2P 119085-07-3P 119085-08-4P 119085-09-5P 119085-10-8P
 119085-11-9P 119085-12-0P 119085-13-1P 119085-14-2P 119085-15-3P
 119085-16-4P 119085-17-5P 119085-18-6P 119085-19-7P 119085-20-0P
 119085-21-1P 119085-22-2P 119085-23-3P 119085-24-4P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except
 adverse); BSU (Biological study, unclassified); SPN (Synthetic
 preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of, as herbicide)
 IT 119084-52-5P 119084-53-6P **119084-54-7P** 119084-55-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for herbicide)
 IT 18438-41-0 118260-49-4 118582-12-0 119084-50-3 119084-51-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, in preparation of herbicide)
 IT **119084-54-7P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as intermediate for herbicide)
 RN 119084-54-7 HCAPLUS
 CN Methanimidamide, N-cyano-N'-(2,3-dihydro-2,2-dimethyl-1H-inden-1-yl)-
 (9CI) (CA INDEX NAME)



L24 ANSWER 18 OF 18 HCAPLUS COPYRIGHT 2005 ACS on STN
 AN 1989:75497 HCAPLUS
 DN 110:75497
 ED Entered STN: 04 Mar 1989
 TI Preparation of tricyclic 1H-imidazole-5-carboxylates as herbicides
 IN Lutz, William R.; Verschueren, Wim G.; Fischer, Hanspeter; Van Lommen, Guy
 R. E.
 PA Janssen Pharmaceutica N. V., Belg.
 SO Eur. Pat. Appl., 29 pp.
 CODEN: EPXXDW
 DT Patent
 LA English
 IC ICM C07D233-90
 ICS C07D401-04; C07D405-04; C07D409-04; A01N043-50
 ICA C07C101-18; C07C103-48; C07C087-455; C07C121-43
 CC 28-9 (Heterocyclic Compounds (More Than One Hetero Atom))
 Section cross-reference(s): 5
 FAN.CNT 1

| | PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----|---|------|----------|-----------------|--------------|
| PI | EP 275603 | A1 | 19880727 | EP 1987-202588 | 19871221 <-- |
| | R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE | | | | |
| | US 4830664 | A | 19890516 | US 1987-134440 | 19871217 <-- |
| | DK 8706821 | A | 19880624 | DK 1987-6821 | 19871222 <-- |
| | JP 63166869 | A2 | 19880711 | JP 1987-323047 | 19871222 <-- |
| | HU 46677 | A2 | 19881128 | HU 1987-5955 | 19871222 <-- |
| | HU 198188 | B | 19890828 | | |
| | ZA 8709613 | A | 19890830 | ZA 1987-9613 | 19871222 <-- |
| | IL 84916 | A1 | 19910718 | IL 1987-84916 | 19871222 <-- |
| | AU 8782976 | A1 | 19880623 | AU 1987-82976 | 19871223 <-- |
| | AU 595085 | B2 | 19900322 | | |
| | BR 8707032 | A | 19880802 | BR 1987-7032 | 19871223 <-- |

US 4927449 A 19900522 US 1988-289947 19881227 <--
 PRAI GB 1986-30759 A 19861223 <--
 US 1987-134440 B3 19871217 <--

CLASS

| PATENT NO. | CLASS | PATENT FAMILY CLASSIFICATION CODES |
|------------|-------|---|
| EP 275603 | ICM | C07D233-90 |
| | ICS | C07D401-04; C07D405-04; C07D409-04; A01N043-50 |
| | ICA | C07C101-18; C07C103-48; C07C087-455; C07C121-43 |

OS MARPAT 110:75497

GI For diagram(s), see printed CA Issue.

AB The title compds. [I; A = alkylene, cycloalkanediyl; R1 = H, SH; R2 = H, alkyl, alkoxyalkyl, arylalkyl, etc.; R3-R6 = halo, (un)substituted alkyl, alkoxy, aryl, etc.; R7, R8 = H, alkyl, alkoxy, halo, etc.; Y = O, SOm, NR9, CH2; R9 = H, alkyl, alkanoyl, 4-MeC6H4SO2; m = 0-2; n = 1-3] were prepared 2,3,3A,8a-tetrahydrocyclopenta[a]inden-8(1H)-one and HCl.cntdot.H2NCH2CO2Me in MeOH containing KOAc and thiophene were hydrogenated over Pd/C to give RNHCH2CO2Me (R = 1,2,3,3a,8,8a-hexahydrocyclopenta[a]inden-8-yl) which was stirred with HCO2H in Ac2O to give RN(CHO)CO2Me. The latter was stirred overnight with HCO2Me in THF containing NaH and the product was stirred overnight at 60.degree. with KSCN and HCl in aqueous MeOH to give cyclopentaindenylimidazole II which gave complete kill of Echinochloa crus galli at 4 kg/ha.

ST imidazolecarboxylate tricyclic prepn herbicide

IT Rice

(herbicides for, tricyclic imidazolecarboxylates)

IT Herbicides

(tricyclic imidazolecarboxylates)

IT 118788-14-0P 118788-15-1P 118788-17-3P 118788-18-4P 118788-20-8P

118788-21-9P 118788-22-0P 118788-23-1P 118788-24-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of herbicides)

IT 118788-12-8P 118788-13-9P 118788-26-4P 118788-27-5P 118788-29-7P

118788-30-0P 118788-32-2P 118788-33-3P 118788-34-4P 118788-35-5P

118788-36-6P 118788-37-7P 118788-38-8P 118788-39-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as herbicide)

IT 96-32-2 1203-67-4 3084-00-2 5680-79-5 65226-98-4 118788-16-2

118788-19-5 118788-23-1 118788-40-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of herbicides)

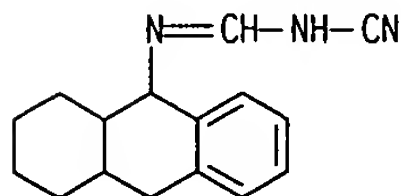
IT 118788-22-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of herbicides)

RN 118788-22-0 HCAPLUS

CN Methanimidamide, N-cyano-N'-(1,2,3,4,4a,9,9a,10-octahydro-9-anthracenyl)-(9CI) (CA INDEX NAME)



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